



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:13 PM GMT

PDB ID : 1EJI
Title : RECOMBINANT SERINE HYDROXYMETHYLTRANSFERASE
(MOUSE)
Authors : Szebenyi, D.M.E.; Liu, X.; Kriksunov, I.A.; Stover, P.J.; Thiel, D.J.
Deposited on : 2000-03-02
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

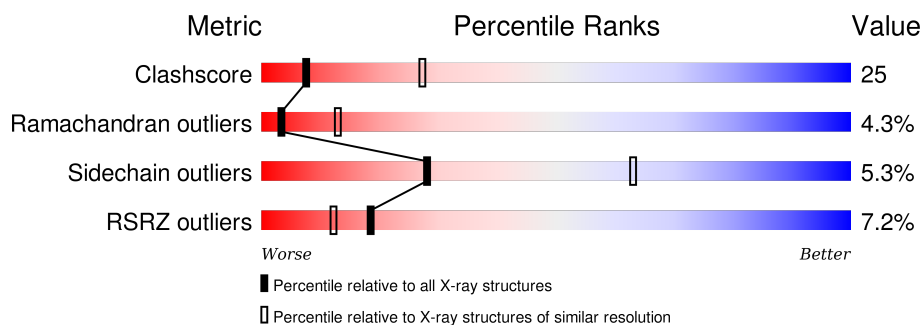
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	478	<div> <div>9%</div> <div>57%</div> <div>38%</div> <div>.</div> </div>
1	B	478	<div> <div>5%</div> <div>59%</div> <div>36%</div> <div>5%</div> <div>.</div> </div>
1	C	478	<div> <div>6%</div> <div>54%</div> <div>38%</div> <div>6%</div> <div>.</div> </div>
1	D	478	<div> <div>8%</div> <div>53%</div> <div>41%</div> <div>.</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	THF	B	601	-	-	-	X
3	THF	D	602	-	-	-	X

2 Entry composition [i](#)

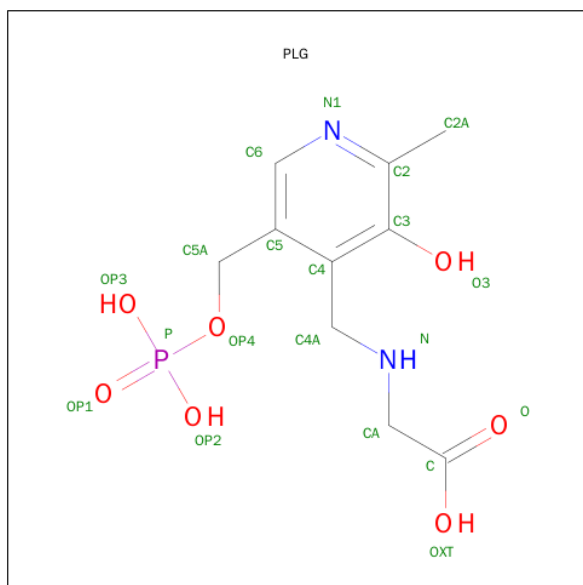
There are 4 unique types of molecules in this entry. The entry contains 14984 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SERINE HYDROXYMETHYLTRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	Se	0	0	0
			3695	2329	641	704	10	11			
1	B	478	Total	C	N	O	S	Se	0	0	0
			3695	2329	641	704	10	11			
1	C	478	Total	C	N	O	S	Se	0	0	0
			3695	2329	641	704	10	11			
1	D	478	Total	C	N	O	S	Se	0	0	0
			3695	2329	641	704	10	11			

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YL-METHANE] (three-letter code: PLG) (formula: $C_{10}H_{15}N_2O_7P$).



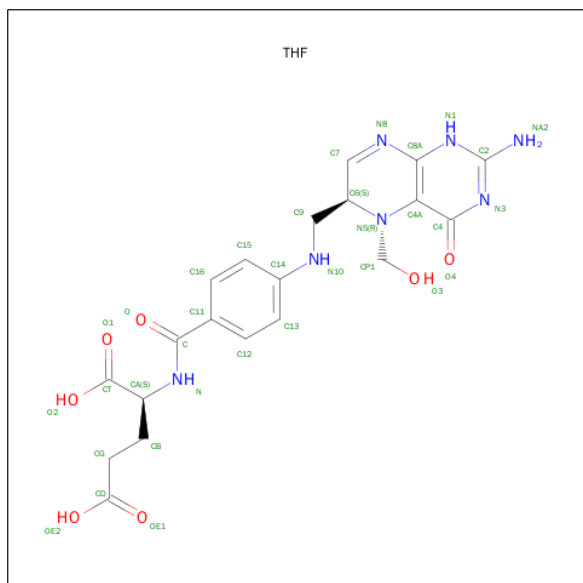
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

- Molecule 3 is 5-HYDROXYMETHYLENE-6-HYDROFOLIC ACID (three-letter code: THF) (formula: $C_{20}H_{23}N_7O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			34	20	7	7		
3	B	1	Total	C	N	O	0	0
			34	20	7	7		
3	D	1	Total	C	N	O	0	0
			34	20	7	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	4	Total	O	0	0
			4	4		
4	C	9	Total	O	0	0
			9	9		
4	D	4	Total	O	0	0
			4	4		

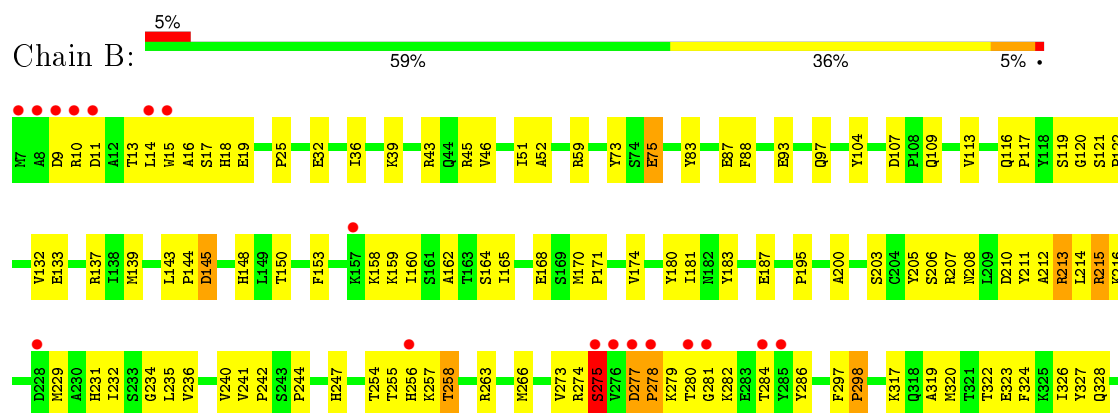
3 Residue-property plots

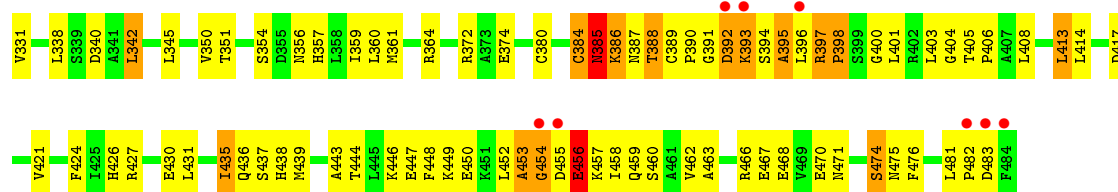
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

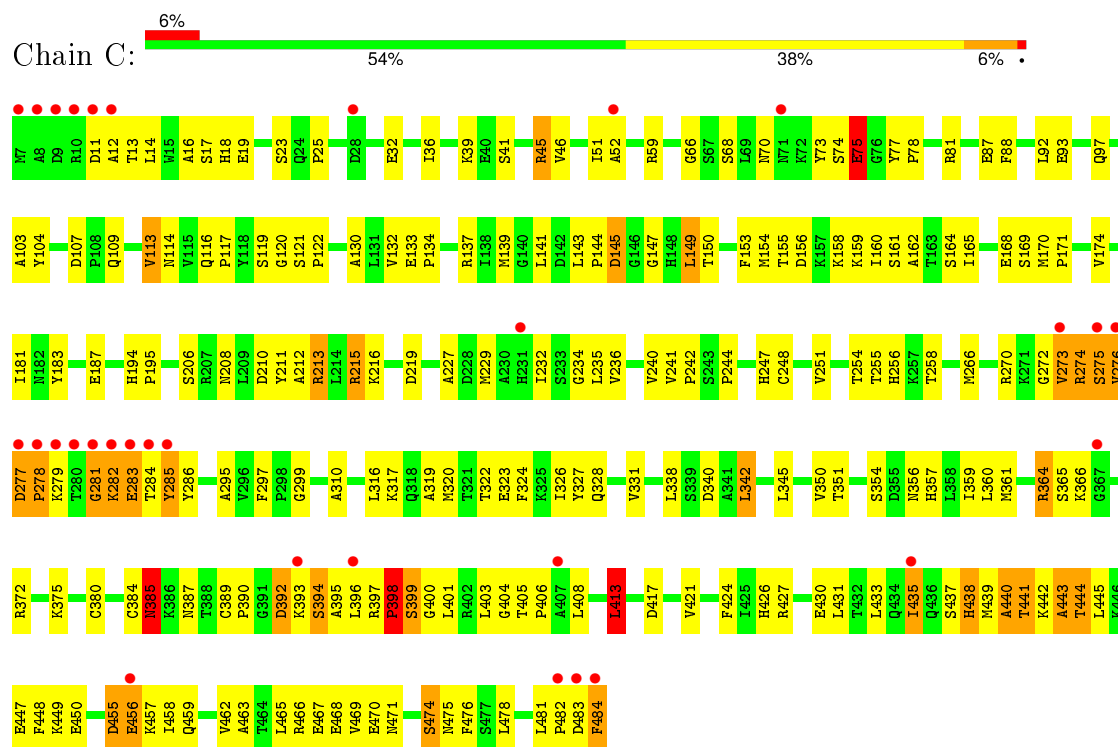


• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

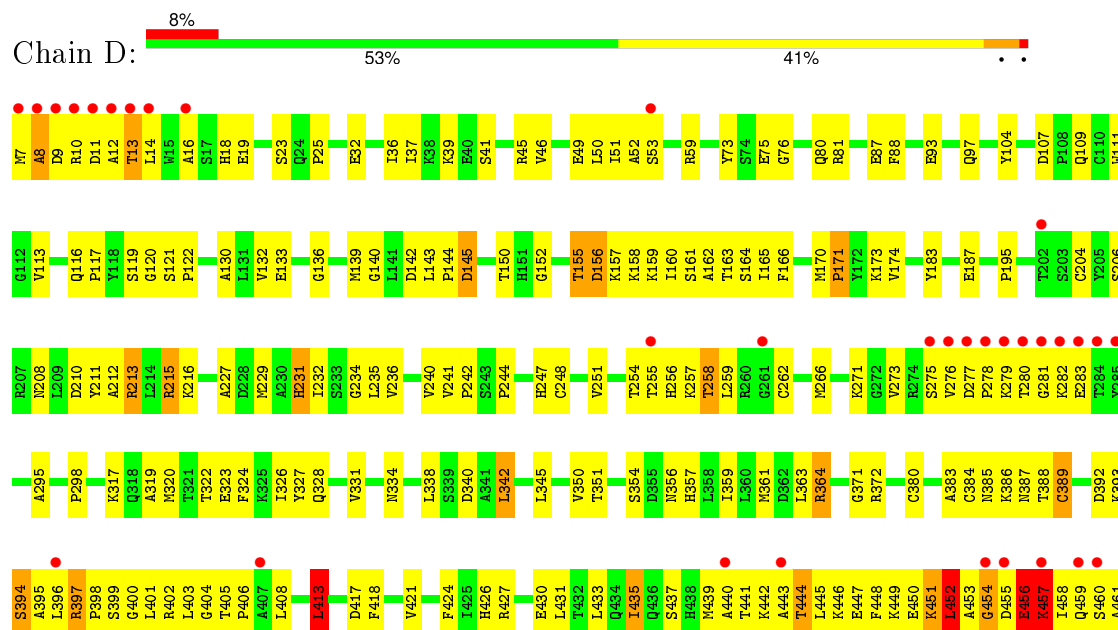




• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE



• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE



V462	A463	L465	R466	E467	E468	V469	E470	N471	F472	A473	S474	N475	F476	L481	P482	D483	F484

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	142.52Å 142.52Å 270.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.10 – 2.90 32.10 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.7 (32.10-2.90) 91.7 (32.10-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.90Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.271 , 0.228 0.265 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	75.1	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 83.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 108428 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14984	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PLG, THF

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/3760	0.68	4/5063 (0.1%)
1	B	0.42	0/3760	0.69	3/5063 (0.1%)
1	C	0.42	0/3760	0.69	4/5063 (0.1%)
1	D	0.40	0/3760	0.69	4/5063 (0.1%)
All	All	0.41	0/15040	0.69	15/20252 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	45	ARG	NE-CZ-NH1	-8.05	116.27	120.30
1	D	45	ARG	NE-CZ-NH2	7.97	124.28	120.30
1	B	45	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	A	45	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	A	45	ARG	NE-CZ-NH1	-7.54	116.53	120.30
1	C	45	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	C	45	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	364	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	C	364	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	B	45	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	D	364	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	364	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	D	364	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	364	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	364	ARG	NE-CZ-NH1	-5.67	117.46	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3695	0	3660	177	0
1	B	3695	0	3660	188	0
1	C	3695	0	3658	218	0
1	D	3695	0	3658	211	0
2	A	20	0	11	1	0
2	B	20	0	11	5	0
2	C	20	0	10	3	0
2	D	20	0	10	2	0
3	A	34	0	21	3	0
3	B	34	0	21	1	0
3	D	34	0	21	1	0
4	A	5	0	0	1	0
4	B	4	0	0	0	0
4	C	9	0	0	2	0
4	D	4	0	0	1	0
All	All	14984	0	14741	754	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (754) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:THR:HG22	1:D:157:LYS:H	1.21	1.04
1:B:280:THR:HB	1:B:282:LYS:HE3	1.40	1.01
1:C:59:ARG:HG3	1:C:481:LEU:HD23	1.47	0.97
1:D:458:ILE:C	1:D:460:SER:H	1.67	0.94
1:A:435:ILE:HD12	1:A:448:PHE:HE1	1.30	0.94
1:A:432:THR:O	1:A:436:GLN:HG2	1.68	0.94
1:C:234:GLY:HA3	1:C:258:THR:O	1.67	0.92
1:C:155:THR:HG23	1:C:158:LYS:H	1.33	0.92
1:D:7:MET:N	1:D:10:ARG:HD3	1.89	0.87
1:D:452:LEU:HD13	1:D:453:ALA:H	1.40	0.87
1:C:384:CYS:O	1:C:385:ASN:HB2	1.74	0.87
1:C:361:MSE:HE2	1:C:403:LEU:HD11	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:VAL:HA	1:C:282:LYS:HB2	1.55	0.86
1:B:456:GLU:HB3	1:B:458:ILE:H	1.41	0.85
1:A:451:LYS:HB3	1:A:458:ILE:HD12	1.60	0.83
1:A:350:VAL:HG12	1:A:351:THR:HG23	1.61	0.83
1:B:456:GLU:CB	1:B:458:ILE:HG22	2.09	0.83
1:D:155:THR:HG22	1:D:157:LYS:N	1.95	0.82
1:D:155:THR:CG2	1:D:157:LYS:H	1.92	0.82
1:C:276:VAL:HG13	1:C:281:GLY:HA2	1.62	0.81
1:C:275:SER:CB	1:C:284:THR:H	1.93	0.81
1:D:52:ALA:HB3	1:D:402:ARG:HH11	1.46	0.81
1:A:435:ILE:HD12	1:A:448:PHE:CE1	2.17	0.80
1:B:361:MSE:HE2	1:B:403:LEU:HD11	1.63	0.80
1:B:279:LYS:N	1:B:279:LYS:HD2	1.97	0.80
1:D:458:ILE:C	1:D:460:SER:N	2.31	0.78
1:A:75:GLU:HG3	1:A:83:TYR:HE2	1.47	0.78
1:D:350:VAL:HG12	1:D:351:THR:HG23	1.63	0.78
1:C:277:ASP:HB3	1:C:278:PRO:HD3	1.66	0.78
1:C:372:ARG:NH2	1:C:443:ALA:HB1	1.99	0.77
1:C:398:PRO:O	1:C:399:SER:HB2	1.84	0.77
1:A:397:ARG:N	1:A:398:PRO:HD3	1.98	0.77
1:B:397:ARG:N	1:B:398:PRO:HD3	1.98	0.77
1:C:145:ASP:OD2	1:C:174:VAL:HG22	1.85	0.77
1:D:435:ILE:HG13	1:D:452:LEU:HD23	1.66	0.76
1:C:444:THR:HG22	1:C:447:GLU:H	1.47	0.76
1:A:361:MSE:HE2	1:A:403:LEU:HD11	1.65	0.76
1:D:361:MSE:HE2	1:D:403:LEU:HD11	1.67	0.75
1:C:350:VAL:HG12	1:C:351:THR:HG23	1.67	0.75
1:C:159:LYS:HD3	1:C:164:SER:O	1.85	0.75
1:D:208:ASN:ND2	1:D:242:PRO:HD2	2.02	0.75
1:D:435:ILE:HD13	1:D:435:ILE:O	1.87	0.75
1:B:372:ARG:HH12	1:B:397:ARG:NH1	1.85	0.74
1:A:120:GLY:HA3	2:A:500:PLG:H5A2	1.69	0.74
1:A:277:ASP:HB3	1:A:280:THR:HG23	1.67	0.74
1:A:387:ASN:HD21	3:A:600:THF:HN1	1.32	0.74
1:D:467:GLU:HG2	1:D:471:ASN:HD21	1.53	0.74
1:A:451:LYS:HE2	1:A:458:ILE:HD11	1.68	0.73
1:B:389:CYS:HB2	1:B:390:PRO:HD2	1.69	0.73
1:D:322:THR:O	1:D:326:ILE:HG22	1.88	0.73
1:B:453:ALA:C	1:B:455:ASP:H	1.90	0.73
1:A:447:GLU:O	1:A:450:GLU:HG2	1.87	0.73
1:A:467:GLU:HG2	1:A:471:ASN:HD21	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:VAL:HG12	1:B:351:THR:HG23	1.70	0.73
1:A:386:LYS:O	1:A:398:PRO:HG2	1.88	0.73
1:C:208:ASN:ND2	1:C:242:PRO:HD2	2.03	0.73
1:D:452:LEU:HD13	1:D:453:ALA:N	2.02	0.73
1:B:456:GLU:HB3	1:B:458:ILE:HG22	1.69	0.73
1:B:208:ASN:ND2	1:B:242:PRO:HD2	2.03	0.73
1:D:452:LEU:CD1	1:D:453:ALA:H	2.02	0.73
1:D:46:VAL:HG12	1:D:474:SER:HB3	1.71	0.73
1:B:456:GLU:HB2	1:B:458:ILE:HG22	1.71	0.72
1:A:435:ILE:O	1:A:435:ILE:HD13	1.89	0.72
1:B:46:VAL:HG12	1:B:474:SER:HB3	1.71	0.72
1:B:387:ASN:HD21	3:B:601:THF:HN1	1.38	0.72
1:A:386:LYS:HE3	1:A:396:LEU:HA	1.71	0.72
1:B:380:CYS:SG	1:B:462:VAL:HG23	2.30	0.72
1:A:208:ASN:ND2	1:A:242:PRO:HD2	2.04	0.72
1:D:447:GLU:O	1:D:451:LYS:HE2	1.90	0.72
1:C:46:VAL:HG12	1:C:474:SER:HB3	1.72	0.71
1:C:459:GLN:HA	1:C:462:VAL:HG12	1.71	0.71
1:B:143:LEU:HD23	1:B:143:LEU:C	2.10	0.71
1:C:93:GLU:O	1:C:97:GLN:HG3	1.91	0.70
1:C:14:LEU:HD12	1:C:14:LEU:H	1.56	0.70
1:A:451:LYS:HE2	1:A:458:ILE:CD1	2.21	0.70
1:B:444:THR:HG23	1:B:447:GLU:OE2	1.92	0.70
1:A:46:VAL:HG12	1:A:474:SER:HB3	1.72	0.70
1:C:467:GLU:HG2	1:C:471:ASN:HD21	1.55	0.70
1:D:255:THR:HG22	1:D:266:MSE:HE2	1.74	0.70
1:D:52:ALA:HB3	1:D:402:ARG:NH1	2.07	0.69
1:A:380:CYS:SG	1:A:462:VAL:HG23	2.32	0.69
1:A:459:GLN:HA	1:A:462:VAL:HG12	1.72	0.69
1:B:322:THR:O	1:B:326:ILE:HG22	1.91	0.69
1:B:158:LYS:HE3	1:B:160:ILE:CD1	2.22	0.69
1:D:240:VAL:HG23	1:D:241:VAL:HG13	1.73	0.69
1:C:187:GLU:OE1	1:C:216:LYS:HE3	1.92	0.69
1:A:361:MSE:HE3	1:A:401:LEU:HB2	1.74	0.69
1:D:7:MET:N	1:D:10:ARG:HH21	1.91	0.69
1:D:380:CYS:SG	1:D:462:VAL:HG23	2.32	0.69
1:A:322:THR:O	1:A:326:ILE:HG22	1.93	0.69
1:A:93:GLU:O	1:A:97:GLN:HG3	1.92	0.68
1:B:235:LEU:HD23	1:B:328:GLN:HG3	1.76	0.68
1:C:443:ALA:O	1:C:444:THR:HB	1.94	0.68
1:C:282:LYS:O	1:C:283:GLU:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:TYR:O	1:D:331:VAL:HG23	1.94	0.68
1:B:274:ARG:O	1:B:284:THR:HB	1.94	0.68
1:A:240:VAL:HG23	1:A:241:VAL:HG13	1.75	0.68
1:A:8:ALA:O	1:A:9:ASP:HB2	1.94	0.67
1:A:277:ASP:HB2	1:A:282:LYS:H	1.59	0.67
1:D:143:LEU:HD11	3:D:602:THF:O4	1.95	0.67
1:D:37:ILE:HG22	1:D:484:PHE:O	1.95	0.67
1:B:454:GLY:HA2	1:B:459:GLN:OE1	1.94	0.67
1:B:467:GLU:HG2	1:B:471:ASN:HD21	1.58	0.67
1:C:441:THR:OG1	1:C:442:LYS:HE3	1.95	0.67
1:C:361:MSE:HE3	1:C:401:LEU:HB2	1.75	0.67
1:B:51:ILE:HG12	1:B:384:CYS:O	1.95	0.66
1:D:120:GLY:HA3	2:D:503:PLG:H5A2	1.77	0.66
1:D:397:ARG:HG3	1:D:397:ARG:HH21	1.60	0.66
1:B:435:ILE:O	1:B:435:ILE:HD13	1.94	0.66
1:C:130:ALA:HB2	1:C:295:ALA:HB2	1.76	0.66
1:C:322:THR:O	1:C:326:ILE:HG22	1.96	0.66
1:A:413:LEU:HD22	1:A:476:PHE:CE2	2.30	0.66
1:A:317:LYS:HA	1:A:320:MSE:HE3	1.77	0.66
1:C:317:LYS:HA	1:C:320:MSE:HE3	1.78	0.66
1:B:317:LYS:HA	1:B:320:MSE:HE3	1.78	0.66
1:B:144:PRO:HB3	1:B:393:LYS:HE2	1.78	0.65
1:C:155:THR:HG22	1:C:158:LYS:O	1.95	0.65
1:C:120:GLY:HA3	2:C:502:PLG:H5A2	1.78	0.65
1:D:386:LYS:HG3	1:D:386:LYS:O	1.95	0.65
1:C:14:LEU:H	1:C:14:LEU:CD1	2.08	0.65
1:C:235:LEU:HD23	1:C:328:GLN:HG3	1.78	0.65
1:B:93:GLU:O	1:B:97:GLN:HG3	1.95	0.65
1:D:467:GLU:HG2	1:D:471:ASN:ND2	2.12	0.65
1:A:467:GLU:HG2	1:A:471:ASN:ND2	2.11	0.65
1:C:380:CYS:SG	1:C:462:VAL:HG23	2.37	0.65
1:C:327:TYR:O	1:C:331:VAL:HG23	1.97	0.65
1:C:445:LEU:HD22	1:C:449:LYS:HE3	1.79	0.64
1:B:459:GLN:HA	1:B:462:VAL:HG12	1.79	0.64
1:A:16:ALA:O	1:A:19:GLU:HB3	1.97	0.64
1:B:274:ARG:HD3	1:B:286:TYR:CE1	2.32	0.64
1:D:450:GLU:O	1:D:452:LEU:N	2.31	0.64
1:B:280:THR:HG22	1:B:281:GLY:H	1.63	0.64
1:C:154:MSE:HE2	1:C:164:SER:HB2	1.80	0.64
1:C:240:VAL:HG23	1:C:241:VAL:HG13	1.79	0.64
1:C:413:LEU:HD22	1:C:476:PHE:CE2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:SER:HB2	1:B:397:ARG:O	1.98	0.63
1:D:317:LYS:HA	1:D:320:MSE:HE3	1.81	0.63
1:A:121:SER:HB2	1:A:122:PRO:HD3	1.80	0.63
1:A:139:MSE:HG3	1:A:195:PRO:HB3	1.80	0.63
1:B:413:LEU:HD22	1:B:476:PHE:CE2	2.33	0.63
1:D:276:VAL:HG12	1:D:283:GLU:HG2	1.80	0.63
1:C:455:ASP:O	1:C:457:LYS:N	2.32	0.62
1:B:435:ILE:C	1:B:435:ILE:HD13	2.19	0.62
1:D:277:ASP:HB3	1:D:280:THR:HB	1.79	0.62
1:A:255:THR:HG22	1:A:266:MSE:HE2	1.81	0.62
1:C:278:PRO:HG2	1:C:282:LYS:HE3	1.81	0.62
1:C:449:LYS:HB2	1:C:449:LYS:NZ	2.14	0.62
1:D:51:ILE:HG13	1:D:383:ALA:HB1	1.81	0.62
1:B:148:HIS:HB2	1:B:203:SER:OG	1.99	0.62
1:D:212:ALA:HA	1:D:247:HIS:CD2	2.35	0.62
1:B:274:ARG:HB3	1:B:286:TYR:CE2	2.34	0.62
1:B:389:CYS:HB2	1:B:390:PRO:CD	2.29	0.62
1:B:240:VAL:HG23	1:B:241:VAL:HG13	1.81	0.62
1:B:453:ALA:O	1:B:455:ASP:N	2.32	0.62
1:D:361:MSE:HE3	1:D:401:LEU:HB2	1.81	0.62
1:C:121:SER:HB2	1:C:122:PRO:HD3	1.81	0.62
1:A:322:THR:HG22	1:B:14:LEU:HD21	1.80	0.62
1:C:467:GLU:HG2	1:C:471:ASN:ND2	2.14	0.61
1:C:322:THR:HG22	1:D:14:LEU:HD11	1.80	0.61
1:C:361:MSE:O	1:C:400:GLY:HA2	2.00	0.61
1:C:16:ALA:O	1:C:19:GLU:HB3	2.00	0.61
1:A:439:MSE:O	1:A:441:THR:HG23	2.01	0.61
1:D:16:ALA:O	1:D:19:GLU:HB3	2.00	0.61
1:D:459:GLN:HA	1:D:462:VAL:HG12	1.83	0.61
1:D:371:GLY:HA2	1:D:386:LYS:HD3	1.82	0.61
1:B:121:SER:HB2	1:B:122:PRO:HD3	1.80	0.61
1:B:277:ASP:C	1:B:279:LYS:H	2.04	0.61
1:D:144:PRO:HA	1:D:388:THR:HG21	1.83	0.60
1:C:372:ARG:HH22	1:C:443:ALA:HB1	1.64	0.60
1:D:395:ALA:C	1:D:397:ARG:H	2.03	0.60
1:C:447:GLU:HA	1:C:447:GLU:OE1	2.01	0.60
1:D:395:ALA:O	1:D:396:LEU:HB2	2.01	0.60
1:C:77:TYR:CE2	1:C:116:GLN:NE2	2.69	0.60
1:B:148:HIS:HE1	1:B:150:THR:HG23	1.66	0.60
1:B:384:CYS:O	1:B:385:ASN:HB2	2.01	0.60
1:D:466:ARG:O	1:D:470:GLU:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:TYR:O	1:A:331:VAL:HG23	2.02	0.60
1:B:431:LEU:O	1:B:431:LEU:HD23	2.01	0.60
1:B:327:TYR:O	1:B:331:VAL:HG23	2.01	0.60
1:D:121:SER:HB2	1:D:122:PRO:HD3	1.83	0.60
1:B:467:GLU:HG2	1:B:471:ASN:ND2	2.16	0.60
1:B:361:MSE:HE3	1:B:401:LEU:HB2	1.84	0.60
1:C:435:ILE:HD13	1:C:435:ILE:O	2.02	0.60
1:C:255:THR:HG22	1:C:266:MSE:HE2	1.84	0.60
1:C:278:PRO:HD2	1:C:282:LYS:HG3	1.82	0.59
1:B:158:LYS:HE3	1:B:160:ILE:HD11	1.84	0.59
1:D:364:ARG:NH2	1:D:392:ASP:OD2	2.35	0.59
1:B:435:ILE:HD12	1:B:448:PHE:CE1	2.36	0.59
1:D:93:GLU:O	1:D:97:GLN:HG3	2.02	0.59
1:D:277:ASP:CG	1:D:278:PRO:HD2	2.22	0.59
1:B:280:THR:CB	1:B:282:LYS:HE3	2.25	0.59
1:C:361:MSE:HE3	1:C:401:LEU:HD12	1.85	0.59
1:B:396:LEU:C	1:B:398:PRO:HD3	2.23	0.59
1:C:345:LEU:HD13	1:C:426:HIS:HB2	1.84	0.59
1:B:16:ALA:O	1:B:19:GLU:HB3	2.01	0.59
1:C:278:PRO:C	1:C:279:LYS:HD3	2.22	0.59
1:C:278:PRO:CG	1:C:282:LYS:HE3	2.32	0.59
1:B:446:LYS:O	1:B:450:GLU:HG2	2.02	0.59
1:A:413:LEU:HD22	1:A:476:PHE:CD2	2.37	0.59
1:D:121:SER:HA	1:D:150:THR:HG21	1.84	0.59
1:D:456:GLU:OE1	1:D:456:GLU:O	2.20	0.59
1:A:435:ILE:C	1:A:435:ILE:HD13	2.23	0.59
1:C:413:LEU:HD22	1:C:476:PHE:CD2	2.37	0.59
1:D:345:LEU:HD13	1:D:426:HIS:HB2	1.85	0.58
1:C:149:LEU:HD11	1:D:298:PRO:HB2	1.85	0.58
1:A:235:LEU:HD23	1:A:328:GLN:HG3	1.85	0.58
1:D:405:THR:H	1:D:406:PRO:HD3	1.69	0.58
1:A:59:ARG:NH2	1:B:25:PRO:HG3	2.18	0.58
1:C:213:ARG:HG3	1:C:213:ARG:HH11	1.68	0.58
1:B:345:LEU:HD13	1:B:426:HIS:HB2	1.85	0.58
1:A:431:LEU:O	1:A:431:LEU:HD23	2.03	0.58
1:C:440:ALA:O	1:C:441:THR:HG23	2.03	0.58
1:A:462:VAL:HG13	1:A:463:ALA:N	2.19	0.58
1:C:155:THR:CG2	1:C:158:LYS:H	2.13	0.58
1:C:394:SER:HB3	1:C:397:ARG:O	2.04	0.58
1:A:345:LEU:HD13	1:A:426:HIS:HB2	1.84	0.58
1:C:273:VAL:O	1:C:285:TYR:HA	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:MSE:CE	1:C:401:LEU:HD12	2.34	0.58
1:D:397:ARG:N	1:D:398:PRO:HD3	2.19	0.58
1:D:413:LEU:HD22	1:D:476:PHE:CE2	2.39	0.57
1:C:444:THR:HG22	1:C:447:GLU:N	2.18	0.57
1:A:206:SER:HA	1:A:356:ASN:HD21	1.69	0.57
1:B:385:ASN:HD22	1:B:385:ASN:C	2.07	0.57
1:D:143:LEU:HB3	1:D:144:PRO:HD3	1.86	0.57
1:D:361:MSE:O	1:D:400:GLY:HA2	2.05	0.57
1:B:431:LEU:O	1:B:435:ILE:HG22	2.05	0.57
1:C:11:ASP:O	1:C:13:THR:N	2.36	0.57
1:B:280:THR:HG22	1:B:281:GLY:N	2.18	0.57
1:D:49:GLU:HA	1:D:383:ALA:HB3	1.86	0.57
1:C:326:ILE:HD13	1:D:14:LEU:HB3	1.86	0.57
1:D:442:LYS:O	1:D:442:LYS:HG2	2.04	0.57
1:D:450:GLU:O	1:D:454:GLY:N	2.36	0.57
1:D:50:LEU:HB2	1:D:383:ALA:O	2.05	0.57
1:B:439:MSE:HE3	1:B:443:ALA:CB	2.34	0.57
1:C:459:GLN:HA	1:C:462:VAL:CG1	2.35	0.57
1:D:187:GLU:OE1	1:D:216:LYS:HE3	2.04	0.57
1:C:75:GLU:HG2	1:C:297:PHE:CZ	2.39	0.57
1:B:256:HIS:O	1:B:257:LYS:HB2	2.03	0.56
1:A:387:ASN:ND2	3:A:600:THF:HN1	2.00	0.56
1:C:59:ARG:HG3	1:C:481:LEU:CD2	2.29	0.56
1:C:143:LEU:HB3	1:C:144:PRO:CD	2.35	0.56
1:D:455:ASP:O	1:D:456:GLU:C	2.43	0.56
1:B:413:LEU:HD22	1:B:476:PHE:CD2	2.40	0.56
1:A:10:ARG:CZ	1:A:10:ARG:HB2	2.35	0.56
1:B:234:GLY:HA3	1:B:258:THR:O	2.05	0.56
1:D:161:SER:O	1:D:165:ILE:HG13	2.05	0.56
1:A:372:ARG:HD3	1:A:436:GLN:OE1	2.05	0.56
1:B:153:PHE:HD2	1:B:160:ILE:HB	1.70	0.56
1:A:405:THR:H	1:A:406:PRO:HD3	1.70	0.56
1:B:277:ASP:O	1:B:279:LYS:N	2.36	0.56
1:C:18:HIS:HB2	1:D:323:GLU:HB3	1.86	0.56
1:C:427:ARG:O	1:C:430:GLU:HB3	2.06	0.56
1:D:158:LYS:HD2	1:D:160:ILE:HD13	1.86	0.56
1:B:162:ALA:HA	1:B:165:ILE:HD12	1.87	0.56
1:A:212:ALA:HA	1:A:247:HIS:CD2	2.41	0.56
1:B:212:ALA:HA	1:B:247:HIS:CD2	2.41	0.56
1:C:212:ALA:HA	1:C:247:HIS:CD2	2.41	0.55
1:A:395:ALA:O	1:A:396:LEU:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:ARG:O	1:C:470:GLU:HG3	2.06	0.55
1:C:405:THR:H	1:C:406:PRO:HD3	1.70	0.55
1:A:187:GLU:OE1	1:A:216:LYS:HE3	2.06	0.55
1:D:235:LEU:HD23	1:D:328:GLN:HG3	1.88	0.55
1:D:51:ILE:HG12	1:D:384:CYS:O	2.06	0.55
1:D:50:LEU:H	1:D:383:ALA:HB3	1.72	0.55
1:A:141:LEU:O	1:A:147:GLY:HA3	2.05	0.55
1:D:458:ILE:HG22	1:D:461:ALA:HB2	1.89	0.55
1:A:386:LYS:CE	1:A:396:LEU:HA	2.35	0.55
1:B:139:MSE:HG3	1:B:195:PRO:HB3	1.89	0.55
1:B:453:ALA:C	1:B:455:ASP:N	2.57	0.55
1:D:462:VAL:HG13	1:D:463:ALA:N	2.21	0.55
1:D:139:MSE:HG3	1:D:195:PRO:HB3	1.87	0.55
1:C:275:SER:HB2	1:C:284:THR:HB	1.89	0.55
1:C:14:LEU:N	1:C:14:LEU:HD12	2.22	0.55
1:B:159:LYS:HD3	1:B:164:SER:O	2.07	0.55
1:D:363:LEU:HD21	1:D:401:LEU:HD11	1.88	0.55
1:D:413:LEU:HD22	1:D:476:PHE:CD2	2.42	0.55
1:B:466:ARG:O	1:B:470:GLU:HG3	2.07	0.55
1:D:435:ILE:C	1:D:435:ILE:HD13	2.26	0.54
1:D:41:SER:HB2	1:D:484:PHE:O	2.07	0.54
1:C:143:LEU:HB3	1:C:144:PRO:HD3	1.88	0.54
1:D:427:ARG:O	1:D:430:GLU:HB3	2.07	0.54
1:B:104:TYR:CZ	1:B:229:MSE:HE1	2.43	0.54
1:C:375:LYS:HG2	1:C:449:LYS:HG2	1.89	0.54
1:A:274:ARG:HB3	1:A:284:THR:O	2.07	0.54
1:B:374:GLU:OE1	1:B:386:LYS:N	2.40	0.54
1:C:277:ASP:O	1:C:278:PRO:O	2.26	0.54
1:D:338:LEU:O	1:D:342:LEU:HB2	2.07	0.54
1:D:213:ARG:HH11	1:D:213:ARG:HG3	1.71	0.54
1:D:111:TRP:C	1:D:271:LYS:HD3	2.28	0.54
1:D:393:LYS:O	1:D:394:SER:HB3	2.05	0.54
1:C:394:SER:O	1:C:395:ALA:HB3	2.08	0.54
1:B:462:VAL:HG13	1:B:463:ALA:N	2.21	0.54
1:A:323:GLU:HB3	1:B:18:HIS:HB2	1.89	0.54
1:A:437:SER:C	1:A:439:MSE:H	2.10	0.54
1:C:405:THR:N	1:C:406:PRO:CD	2.71	0.54
1:A:66:GLY:O	1:B:481:LEU:HD11	2.08	0.54
1:A:451:LYS:HA	1:A:455:ASP:HB2	1.89	0.54
1:A:405:THR:N	1:A:406:PRO:CD	2.71	0.54
1:A:215:ARG:HG3	1:A:247:HIS:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ARG:O	1:A:470:GLU:HG3	2.08	0.54
1:A:431:LEU:O	1:A:435:ILE:HG22	2.07	0.53
1:A:438:HIS:O	1:A:451:LYS:NZ	2.40	0.53
1:A:277:ASP:CB	1:A:280:THR:HG23	2.36	0.53
1:C:462:VAL:HG13	1:C:463:ALA:N	2.23	0.53
1:B:255:THR:HG22	1:B:266:MSE:HE2	1.89	0.53
1:C:338:LEU:O	1:C:342:LEU:HB2	2.08	0.53
1:D:471:ASN:O	1:D:475:ASN:ND2	2.41	0.53
1:B:427:ARG:O	1:B:430:GLU:HB3	2.08	0.53
1:A:213:ARG:HG3	1:A:213:ARG:HH11	1.71	0.53
1:C:104:TYR:CZ	1:C:229:MSE:HE1	2.43	0.53
1:C:14:LEU:HD23	1:D:322:THR:HG22	1.89	0.53
1:C:235:LEU:HD23	1:C:328:GLN:CG	2.38	0.53
1:D:457:LYS:HA	1:D:457:LYS:HE3	1.90	0.53
1:B:405:THR:H	1:B:406:PRO:HD3	1.72	0.53
1:D:431:LEU:HD23	1:D:431:LEU:O	2.08	0.53
1:D:215:ARG:HG3	1:D:247:HIS:HB3	1.90	0.53
1:C:439:MSE:O	1:C:440:ALA:O	2.27	0.53
1:D:405:THR:N	1:D:406:PRO:CD	2.72	0.53
1:A:338:LEU:O	1:A:342:LEU:HB2	2.09	0.53
1:C:398:PRO:O	1:C:399:SER:CB	2.57	0.53
1:C:154:MSE:HE1	4:C:527:HOH:O	2.09	0.53
1:C:439:MSE:O	1:C:440:ALA:C	2.46	0.52
1:B:393:LYS:HG3	1:B:393:LYS:O	2.09	0.52
1:A:10:ARG:NH2	1:A:10:ARG:HB2	2.24	0.52
1:D:232:ILE:O	1:D:236:VAL:HG23	2.09	0.52
1:C:433:LEU:O	1:C:437:SER:N	2.41	0.52
1:D:431:LEU:O	1:D:435:ILE:HG22	2.09	0.52
1:A:10:ARG:NH1	1:B:414:LEU:HD11	2.24	0.52
1:D:405:THR:N	1:D:406:PRO:HD3	2.25	0.52
1:A:424:PHE:HE1	1:A:468:GLU:HG2	1.74	0.52
1:B:279:LYS:N	1:B:279:LYS:CD	2.69	0.52
1:D:10:ARG:C	1:D:12:ALA:H	2.13	0.52
1:C:275:SER:CB	1:C:284:THR:N	2.69	0.52
1:C:74:SER:HB2	1:C:81:ARG:NH1	2.25	0.52
1:D:130:ALA:HB2	1:D:295:ALA:HB2	1.91	0.52
1:B:405:THR:N	1:B:406:PRO:CD	2.73	0.52
1:A:107:ASP:OD2	1:A:109:GLN:HB2	2.10	0.52
1:D:456:GLU:OE1	1:D:458:ILE:N	2.36	0.52
1:B:455:ASP:O	1:B:456:GLU:CB	2.58	0.52
1:A:256:HIS:O	1:A:257:LYS:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:LEU:O	1:B:342:LEU:HB2	2.10	0.52
1:C:141:LEU:O	1:C:147:GLY:HA3	2.10	0.52
1:D:143:LEU:HB3	1:D:144:PRO:CD	2.39	0.51
1:B:104:TYR:CE2	1:B:229:MSE:HE1	2.44	0.51
1:C:392:ASP:OD2	1:C:399:SER:HB2	2.10	0.51
1:D:445:LEU:HD11	1:D:446:LYS:HE3	1.91	0.51
1:A:481:LEU:HB3	1:A:482:PRO:CD	2.40	0.51
1:C:153:PHE:HD2	1:C:160:ILE:HB	1.75	0.51
1:B:357:HIS:HD1	1:B:357:HIS:H	1.57	0.51
1:C:41:SER:HB2	1:C:484:PHE:O	2.10	0.51
1:B:277:ASP:N	1:B:278:PRO:HD3	2.26	0.51
1:B:9:ASP:O	1:B:11:ASP:N	2.42	0.51
1:C:130:ALA:HB2	1:C:295:ALA:CB	2.40	0.51
1:C:275:SER:O	1:C:276:VAL:O	2.29	0.51
1:A:427:ARG:O	1:A:430:GLU:HB3	2.11	0.51
1:C:32:GLU:O	1:C:36:ILE:HG13	2.11	0.51
1:D:159:LYS:HD3	1:D:164:SER:O	2.10	0.51
1:D:206:SER:HA	1:D:356:ASN:HD21	1.76	0.51
1:A:385:ASN:OD1	1:A:402:ARG:NH2	2.39	0.51
1:A:413:LEU:HD13	1:A:417:ASP:HB3	1.92	0.51
1:C:254:THR:HB	1:C:256:HIS:CE1	2.46	0.51
1:B:213:ARG:HG3	1:B:213:ARG:HH11	1.75	0.51
1:D:439:MSE:HE2	1:D:443:ALA:CB	2.40	0.50
1:B:32:GLU:O	1:B:36:ILE:HG13	2.10	0.50
1:C:431:LEU:O	1:C:435:ILE:HG22	2.11	0.50
1:C:74:SER:HB2	1:C:81:ARG:HH11	1.76	0.50
1:C:274:ARG:HG2	1:C:286:TYR:OH	2.10	0.50
1:B:206:SER:HA	1:B:356:ASN:HD21	1.76	0.50
1:A:154:MSE:HE3	1:A:159:LYS:HG2	1.93	0.50
1:A:204:CYS:SG	1:A:387:ASN:OD1	2.64	0.50
1:C:471:ASN:O	1:C:475:ASN:ND2	2.45	0.50
1:B:235:LEU:HD23	1:B:328:GLN:CG	2.40	0.50
1:B:413:LEU:HD13	1:B:417:ASP:HB3	1.91	0.50
1:D:413:LEU:HD13	1:D:417:ASP:HB3	1.93	0.50
1:D:231:HIS:HD2	1:D:357:HIS:NE2	2.09	0.50
1:A:232:ILE:O	1:A:236:VAL:HG23	2.11	0.50
1:D:450:GLU:O	1:D:454:GLY:HA3	2.12	0.50
1:D:459:GLN:CA	1:D:462:VAL:HG12	2.42	0.50
1:C:104:TYR:CE2	1:C:229:MSE:HE1	2.47	0.50
1:A:450:GLU:C	1:A:452:LEU:N	2.65	0.50
1:A:389:CYS:O	1:A:391:GLY:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:MSE:HG3	1:C:195:PRO:HB3	1.93	0.50
1:A:211:TYR:CZ	1:A:244:PRO:HB3	2.46	0.50
1:C:282:LYS:O	1:C:283:GLU:CB	2.60	0.49
1:B:254:THR:HB	1:B:256:HIS:CE1	2.47	0.49
1:C:435:ILE:C	1:C:435:ILE:HD13	2.32	0.49
1:B:452:LEU:O	1:B:452:LEU:HD13	2.11	0.49
1:C:431:LEU:O	1:C:431:LEU:HD23	2.12	0.49
1:C:405:THR:N	1:C:406:PRO:HD3	2.27	0.49
1:D:9:ASP:O	1:D:13:THR:HB	2.13	0.49
1:C:215:ARG:HG3	1:C:247:HIS:HB3	1.93	0.49
1:A:442:LYS:O	1:A:442:LYS:HG2	2.13	0.49
1:C:323:GLU:HA	1:D:14:LEU:HD12	1.94	0.49
1:C:274:ARG:HH11	1:C:274:ARG:HG2	1.76	0.49
1:D:424:PHE:HE1	1:D:468:GLU:HG2	1.76	0.49
1:A:374:GLU:OE1	1:A:386:LYS:N	2.45	0.49
1:C:273:VAL:HG12	1:C:274:ARG:N	2.28	0.49
1:A:424:PHE:CE1	1:A:468:GLU:HG2	2.47	0.49
1:D:424:PHE:CE1	1:D:468:GLU:HG2	2.47	0.49
1:D:450:GLU:C	1:D:452:LEU:N	2.66	0.49
1:D:162:ALA:HA	1:D:165:ILE:HD12	1.95	0.49
1:B:384:CYS:O	1:B:385:ASN:CB	2.60	0.49
1:C:413:LEU:HD13	1:C:417:ASP:HB3	1.95	0.49
1:C:150:THR:HG22	4:D:526:HOH:O	2.13	0.49
1:D:384:CYS:HB3	1:D:385:ASN:H	1.50	0.48
1:C:206:SER:HA	1:C:356:ASN:HD21	1.78	0.48
1:B:449:LYS:HB2	1:B:449:LYS:NZ	2.28	0.48
1:D:389:CYS:N	1:D:392:ASP:OD1	2.45	0.48
1:A:25:PRO:HG3	1:B:59:ARG:NH2	2.28	0.48
1:D:227:ALA:HB2	1:D:248:CYS:SG	2.54	0.48
1:C:107:ASP:OD2	1:C:109:GLN:HB2	2.13	0.48
1:B:395:ALA:C	1:B:397:ARG:H	2.16	0.48
1:B:397:ARG:N	1:B:398:PRO:CD	2.71	0.48
1:C:456:GLU:O	1:C:457:LYS:C	2.52	0.48
1:B:132:VAL:O	1:B:133:GLU:HB2	2.13	0.48
1:D:107:ASP:OD2	1:D:109:GLN:HB2	2.13	0.48
1:C:392:ASP:HB2	1:C:394:SER:OG	2.14	0.48
1:D:397:ARG:NH2	1:D:397:ARG:HG3	2.26	0.48
1:B:187:GLU:OE1	1:B:216:LYS:HE3	2.14	0.48
1:D:385:ASN:HB2	1:D:402:ARG:HB3	1.94	0.48
1:B:431:LEU:C	1:B:431:LEU:HD23	2.33	0.48
1:C:235:LEU:CD2	1:C:328:GLN:HG3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:TYR:CD2	1:C:116:GLN:NE2	2.81	0.48
1:C:424:PHE:HE1	1:C:468:GLU:HG2	1.78	0.48
1:A:471:ASN:O	1:A:475:ASN:ND2	2.46	0.48
1:A:59:ARG:HG3	1:A:481:LEU:HD23	1.95	0.48
1:B:263:ARG:HG2	1:B:263:ARG:HH11	1.78	0.48
1:A:450:GLU:C	1:A:452:LEU:H	2.16	0.48
1:C:417:ASP:O	1:C:421:VAL:HG23	2.13	0.48
1:A:18:HIS:CD2	1:B:327:TYR:HB2	2.48	0.48
1:D:357:HIS:H	1:D:357:HIS:HD1	1.62	0.48
1:D:204:CYS:SG	1:D:387:ASN:ND2	2.87	0.48
1:B:361:MSE:O	1:B:400:GLY:HA2	2.13	0.47
1:B:148:HIS:CE1	1:B:150:THR:H	2.32	0.47
1:A:234:GLY:HA3	1:A:258:THR:O	2.14	0.47
1:A:450:GLU:O	1:A:452:LEU:N	2.47	0.47
1:A:326:ILE:HG21	1:B:14:LEU:HD23	1.95	0.47
1:C:270:ARG:NH1	1:C:274:ARG:NH1	2.63	0.47
1:D:32:GLU:O	1:D:36:ILE:HG13	2.14	0.47
1:C:66:GLY:O	1:D:481:LEU:CD1	2.62	0.47
1:C:275:SER:HB3	1:C:284:THR:H	1.74	0.47
1:A:51:ILE:HG12	1:A:384:CYS:HA	1.96	0.47
1:C:365:SER:O	1:C:366:LYS:HG2	2.13	0.47
1:B:143:LEU:CD2	1:B:143:LEU:C	2.82	0.47
1:D:447:GLU:N	1:D:447:GLU:OE2	2.46	0.47
1:B:14:LEU:O	1:B:17:SER:N	2.47	0.47
1:C:213:ARG:CG	1:C:213:ARG:HH11	2.26	0.47
1:B:439:MSE:HE3	1:B:443:ALA:HB1	1.96	0.47
1:D:445:LEU:O	1:D:449:LYS:HB2	2.14	0.47
1:A:405:THR:N	1:A:406:PRO:HD3	2.29	0.47
1:C:424:PHE:CE1	1:C:468:GLU:HG2	2.50	0.47
1:C:319:ALA:HA	1:C:324:PHE:CG	2.50	0.47
1:A:366:LYS:O	1:A:433:LEU:HD11	2.15	0.47
1:D:104:TYR:CE2	1:D:229:MSE:HE1	2.50	0.47
1:A:445:LEU:H	1:A:445:LEU:HD13	1.80	0.47
1:A:431:LEU:C	1:A:431:LEU:HD23	2.35	0.47
1:B:471:ASN:O	1:B:475:ASN:ND2	2.48	0.47
1:C:270:ARG:HH12	1:C:274:ARG:HD3	1.80	0.47
1:D:116:GLN:N	1:D:117:PRO:CD	2.77	0.47
1:D:465:LEU:O	1:D:469:VAL:HG23	2.15	0.47
1:B:211:TYR:CZ	1:B:244:PRO:HB3	2.49	0.47
1:C:455:ASP:OD2	1:C:458:ILE:HG13	2.14	0.47
1:B:215:ARG:HG3	1:B:247:HIS:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:PRO:HG3	1:D:59:ARG:NH2	2.30	0.47
1:B:459:GLN:HA	1:B:462:VAL:CG1	2.45	0.47
1:D:281:GLY:O	1:D:283:GLU:HG3	2.14	0.47
1:D:235:LEU:HD23	1:D:328:GLN:CG	2.45	0.47
1:D:235:LEU:HD23	1:D:328:GLN:NE2	2.30	0.47
1:A:263:ARG:NH1	4:A:510:HOH:O	2.45	0.47
1:D:208:ASN:HD22	1:D:242:PRO:HD2	1.76	0.46
1:C:23:SER:O	1:D:59:ARG:HD3	2.15	0.46
1:D:279:LYS:O	1:D:279:LYS:HG2	2.14	0.46
1:B:447:GLU:HA	1:B:450:GLU:CG	2.45	0.46
1:A:388:THR:HA	1:A:398:PRO:HB3	1.98	0.46
1:B:143:LEU:O	1:B:143:LEU:HD23	2.14	0.46
1:C:78:PRO:HG3	1:C:81:ARG:HH21	1.80	0.46
1:A:145:ASP:OD2	1:A:174:VAL:HG22	2.16	0.46
1:D:80:GLN:HG3	1:D:80:GLN:O	2.14	0.46
1:C:459:GLN:CA	1:C:462:VAL:HG12	2.44	0.46
1:C:51:ILE:HA	4:C:525:HOH:O	2.15	0.46
1:A:104:TYR:CZ	1:A:229:MSE:HE1	2.50	0.46
1:A:397:ARG:N	1:A:398:PRO:CD	2.74	0.46
1:C:174:VAL:HG21	1:C:390:PRO:HG3	1.98	0.46
1:D:433:LEU:O	1:D:437:SER:N	2.44	0.46
1:C:235:LEU:HD23	1:C:328:GLN:NE2	2.31	0.46
1:D:364:ARG:HB2	1:D:399:SER:HB3	1.97	0.46
1:D:227:ALA:HB3	1:D:251:VAL:HG22	1.98	0.46
1:A:235:LEU:HD23	1:A:328:GLN:NE2	2.30	0.46
1:D:213:ARG:CG	1:D:213:ARG:HH11	2.28	0.46
1:D:211:TYR:CZ	1:D:244:PRO:HB3	2.50	0.46
1:A:395:ALA:O	1:A:396:LEU:CB	2.62	0.46
1:D:393:LYS:O	1:D:394:SER:CB	2.63	0.46
1:A:77:TYR:C	1:A:79:GLY:N	2.69	0.46
1:C:275:SER:OG	1:C:276:VAL:N	2.47	0.46
1:B:274:ARG:HB3	1:B:286:TYR:CZ	2.50	0.46
1:C:132:VAL:O	1:C:133:GLU:HB2	2.15	0.46
1:A:116:GLN:N	1:A:117:PRO:CD	2.79	0.46
1:C:155:THR:HG23	1:C:158:LYS:N	2.16	0.46
1:D:10:ARG:HB3	1:D:10:ARG:CZ	2.45	0.45
1:A:275:SER:HB3	1:A:284:THR:OG1	2.17	0.45
1:D:481:LEU:O	1:D:483:ASP:N	2.48	0.45
1:D:104:TYR:CZ	1:D:229:MSE:HE1	2.51	0.45
1:B:424:PHE:HE1	1:B:468:GLU:HG2	1.80	0.45
1:B:200:ALA:HB2	1:B:214:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:LEU:O	1:C:17:SER:N	2.50	0.45
1:A:323:GLU:OE1	1:A:323:GLU:N	2.45	0.45
1:B:263:ARG:HG2	1:B:263:ARG:NH1	2.31	0.45
1:B:183:TYR:CE2	1:B:210:ASP:HB3	2.50	0.45
1:C:59:ARG:NH2	1:D:25:PRO:HG3	2.31	0.45
1:D:155:THR:CG2	1:D:156:ASP:N	2.78	0.45
1:B:280:THR:O	1:B:282:LYS:N	2.47	0.45
1:D:444:THR:HG23	1:D:447:GLU:CD	2.36	0.45
1:A:361:MSE:O	1:A:400:GLY:HA2	2.16	0.45
1:A:207:ARG:NH1	1:A:355:ASP:OD2	2.48	0.45
1:C:232:ILE:O	1:C:236:VAL:HG23	2.17	0.45
1:A:327:TYR:HB2	1:B:18:HIS:CD2	2.52	0.45
1:A:10:ARG:C	1:A:12:ALA:H	2.19	0.45
1:A:272:GLY:O	1:A:274:ARG:N	2.49	0.45
1:B:405:THR:N	1:B:406:PRO:HD3	2.30	0.45
1:D:439:MSE:HE2	1:D:443:ALA:HB1	1.97	0.45
1:A:39:LYS:HB3	1:B:88:PHE:CE1	2.52	0.45
1:D:234:GLY:HA3	1:D:258:THR:O	2.17	0.45
1:B:52:ALA:HA	1:B:404:GLY:HA3	1.99	0.45
1:A:302:GLY:HA3	2:B:501:PLG:OP1	2.16	0.45
1:D:277:ASP:CB	1:D:280:THR:HB	2.46	0.45
1:B:391:GLY:O	1:B:392:ASP:HB2	2.17	0.45
1:C:413:LEU:H	1:C:413:LEU:CD2	2.30	0.45
1:D:372:ARG:HH11	1:D:372:ARG:HG3	1.81	0.45
1:C:70:ASN:HD21	1:D:262:CYS:HA	1.81	0.45
1:A:227:ALA:HB2	1:A:248:CYS:SG	2.57	0.45
1:D:458:ILE:HG22	1:D:458:ILE:O	2.17	0.45
1:A:7:MET:C	1:A:9:ASP:H	2.19	0.45
1:C:408:LEU:HB3	1:C:413:LEU:HG	1.99	0.45
1:B:408:LEU:HB3	1:B:413:LEU:HG	1.98	0.45
1:A:59:ARG:CZ	1:B:25:PRO:HG3	2.47	0.45
1:B:424:PHE:CE1	1:B:468:GLU:HG2	2.52	0.45
1:B:257:LYS:HZ2	2:B:501:PLG:H4A2	1.81	0.45
1:C:393:LYS:O	1:C:394:SER:C	2.55	0.45
1:C:208:ASN:HD22	1:C:242:PRO:HD2	1.78	0.45
1:A:11:ASP:O	1:A:12:ALA:C	2.55	0.45
1:D:132:VAL:O	1:D:133:GLU:HB2	2.17	0.45
1:D:319:ALA:HA	1:D:324:PHE:CG	2.52	0.44
1:C:211:TYR:CZ	1:C:244:PRO:HB3	2.52	0.44
1:C:278:PRO:O	1:C:279:LYS:HD3	2.18	0.44
1:C:456:GLU:O	1:C:459:GLN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:THR:HG22	1:D:282:LYS:HG3	1.99	0.44
1:C:273:VAL:CA	1:C:285:TYR:HA	2.47	0.44
1:A:323:GLU:HG2	1:B:17:SER:HB2	1.99	0.44
1:B:116:GLN:N	1:B:117:PRO:CD	2.80	0.44
1:D:120:GLY:HA3	2:D:503:PLG:C5A	2.47	0.44
1:A:181:ILE:HB	1:A:183:TYR:CE1	2.52	0.44
1:A:181:ILE:HG13	1:A:205:TYR:CZ	2.52	0.44
1:C:354:SER:HB2	1:C:359:ILE:HG22	1.98	0.44
1:A:157:LYS:HD3	1:A:157:LYS:O	2.17	0.44
1:A:137:ARG:HA	1:A:168:GLU:O	2.18	0.44
1:A:208:ASN:HD22	1:A:242:PRO:HD2	1.79	0.44
1:C:435:ILE:HD12	1:C:448:PHE:CE1	2.53	0.44
1:B:277:ASP:C	1:B:279:LYS:N	2.71	0.44
1:A:387:ASN:ND2	3:A:600:THF:N1	2.63	0.44
1:C:270:ARG:NH1	1:C:274:ARG:HD3	2.32	0.44
1:D:417:ASP:O	1:D:421:VAL:HG23	2.17	0.44
1:B:145:ASP:OD2	1:B:174:VAL:HG22	2.17	0.44
1:C:465:LEU:O	1:C:469:VAL:HG23	2.18	0.44
1:B:181:ILE:HG13	1:B:205:TYR:CZ	2.53	0.44
1:B:444:THR:OG1	1:B:447:GLU:HG3	2.18	0.44
1:B:208:ASN:HD22	1:B:242:PRO:HD2	1.80	0.44
1:C:68:SER:HB3	1:D:484:PHE:OXT	2.18	0.44
1:B:180:TYR:CE1	1:B:207:ARG:HG3	2.52	0.44
1:D:10:ARG:CB	1:D:10:ARG:NH2	2.81	0.44
1:B:235:LEU:CD2	1:B:328:GLN:HG3	2.47	0.44
1:D:280:THR:HG21	1:D:282:LYS:HD2	2.00	0.44
1:A:235:LEU:HD23	1:A:328:GLN:CG	2.46	0.44
1:C:299:GLY:O	1:D:162:ALA:HB2	2.18	0.44
1:C:215:ARG:HH11	1:C:219:ASP:CG	2.21	0.44
1:A:213:ARG:HH11	1:A:213:ARG:CG	2.31	0.44
1:D:450:GLU:O	1:D:451:LYS:C	2.56	0.44
1:C:364:ARG:NH2	1:C:392:ASP:OD2	2.50	0.44
1:C:116:GLN:N	1:C:117:PRO:CD	2.80	0.44
1:A:481:LEU:O	1:A:483:ASP:N	2.48	0.44
1:C:273:VAL:HA	1:C:285:TYR:HA	2.00	0.44
1:C:183:TYR:CE2	1:C:210:ASP:HB3	2.52	0.44
1:C:158:LYS:HE2	1:C:158:LYS:HB3	1.91	0.43
1:B:455:ASP:O	1:B:456:GLU:HG2	2.18	0.43
1:C:396:LEU:C	1:C:398:PRO:HD3	2.38	0.43
1:C:154:MSE:HE3	1:C:169:SER:OG	2.18	0.43
1:B:350:VAL:HG21	1:B:360:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:LEU:C	1:D:398:PRO:HD3	2.37	0.43
1:B:119:SER:C	1:B:122:PRO:HD2	2.39	0.43
1:C:92:LEU:HD11	1:C:310:ALA:HA	2.00	0.43
1:C:360:LEU:HD21	1:C:389:CYS:HB3	1.99	0.43
1:B:372:ARG:NH1	1:B:397:ARG:NH1	2.59	0.43
1:A:459:GLN:HA	1:A:462:VAL:CG1	2.43	0.43
1:A:78:PRO:HG2	1:A:93:GLU:HG2	2.00	0.43
1:B:413:LEU:H	1:B:413:LEU:CD2	2.30	0.43
1:D:152:GLY:HA2	1:D:163:THR:HB	1.99	0.43
1:D:144:PRO:HA	1:D:388:THR:CG2	2.48	0.43
1:A:417:ASP:O	1:A:421:VAL:HG23	2.19	0.43
1:C:121:SER:N	1:C:122:PRO:CD	2.82	0.43
1:A:437:SER:C	1:A:439:MSE:N	2.72	0.43
1:D:413:LEU:H	1:D:413:LEU:CD2	2.31	0.43
1:A:299:GLY:O	1:B:162:ALA:HB2	2.18	0.43
1:D:145:ASP:OD2	1:D:174:VAL:HG22	2.19	0.43
1:D:450:GLU:O	1:D:454:GLY:CA	2.65	0.43
1:D:441:THR:C	1:D:443:ALA:H	2.22	0.43
1:B:361:MSE:HE2	1:B:403:LEU:CD1	2.43	0.43
1:C:392:ASP:HB2	1:C:394:SER:CB	2.49	0.43
1:B:372:ARG:HG3	1:B:372:ARG:HH11	1.82	0.43
1:C:120:GLY:HA3	2:C:502:PLG:C5A	2.48	0.43
1:B:121:SER:N	1:B:122:PRO:CD	2.82	0.43
1:C:66:GLY:O	1:D:481:LEU:HD12	2.18	0.43
1:C:319:ALA:HA	1:C:324:PHE:CD2	2.53	0.43
1:A:52:ALA:HA	1:A:404:GLY:HA3	2.00	0.43
1:B:450:GLU:O	1:B:453:ALA:N	2.50	0.43
1:C:357:HIS:H	1:C:357:HIS:HD1	1.65	0.43
1:B:232:ILE:O	1:B:236:VAL:HG23	2.18	0.43
1:D:431:LEU:HD23	1:D:431:LEU:C	2.39	0.43
1:B:447:GLU:HA	1:B:450:GLU:HG2	2.01	0.43
1:B:274:ARG:O	1:B:275:SER:CB	2.66	0.43
1:C:134:PRO:HG3	1:D:166:PHE:CE1	2.53	0.43
1:C:162:ALA:HA	1:C:165:ILE:HD12	2.01	0.43
1:C:316:LEU:HD23	1:C:316:LEU:HA	1.90	0.43
1:B:11:ASP:C	1:B:13:THR:H	2.22	0.43
1:D:119:SER:C	1:D:122:PRO:HD2	2.39	0.43
1:B:43:ARG:HG2	1:B:43:ARG:NH1	2.34	0.43
1:A:119:SER:C	1:A:122:PRO:HD2	2.38	0.43
1:C:52:ALA:HA	1:C:404:GLY:HA3	2.01	0.43
1:C:113:VAL:HG12	1:C:114:ASN:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:ARG:O	1:D:12:ALA:N	2.52	0.43
1:B:257:LYS:NZ	2:B:501:PLG:C4A	2.82	0.43
1:A:280:THR:O	1:A:282:LYS:N	2.52	0.43
1:A:462:VAL:HG13	1:A:463:ALA:H	1.85	0.42
1:B:159:LYS:HD3	1:B:165:ILE:HA	2.01	0.42
1:D:142:ASP:HB3	1:D:145:ASP:HB2	2.00	0.42
1:D:76:GLY:HA3	1:D:81:ARG:HA	2.01	0.42
1:C:435:ILE:CG1	1:C:458:ILE:HD13	2.49	0.42
1:D:319:ALA:HA	1:D:324:PHE:CD2	2.54	0.42
1:A:183:TYR:CE2	1:A:210:ASP:HB3	2.54	0.42
1:C:154:MSE:HG3	1:C:154:MSE:O	2.18	0.42
1:D:334:ASN:HB3	1:D:418:PHE:CE2	2.55	0.42
1:B:297:PHE:CD1	1:B:298:PRO:HA	2.54	0.42
1:C:441:THR:O	1:C:443:ALA:N	2.51	0.42
1:C:14:LEU:CD2	1:D:322:THR:HG22	2.50	0.42
1:D:143:LEU:N	1:D:144:PRO:HD2	2.34	0.42
1:C:327:TYR:HB2	1:D:18:HIS:CD2	2.55	0.42
1:B:139:MSE:HE3	1:B:170:MSE:CE	2.49	0.42
1:A:342:LEU:HA	1:A:342:LEU:HD12	1.88	0.42
1:B:213:ARG:CG	1:B:213:ARG:HH11	2.32	0.42
1:A:156:ASP:HA	1:C:194:HIS:CD2	2.53	0.42
1:A:323:GLU:O	1:A:326:ILE:HG23	2.20	0.42
1:D:334:ASN:HB3	1:D:418:PHE:CD2	2.55	0.42
1:A:354:SER:HB2	1:A:359:ILE:HG22	2.01	0.42
1:A:170:MSE:HE1	1:A:189:ASN:HB3	2.02	0.42
1:A:80:GLN:HG3	1:A:80:GLN:O	2.19	0.42
1:A:319:ALA:HA	1:A:324:PHE:CG	2.54	0.42
1:D:451:LYS:HA	1:D:455:ASP:OD2	2.20	0.42
1:B:417:ASP:O	1:B:421:VAL:HG23	2.20	0.42
1:C:342:LEU:HA	1:C:342:LEU:HD12	1.88	0.42
1:C:139:MSE:HE3	1:C:170:MSE:CE	2.49	0.42
1:C:88:PHE:CE1	1:D:39:LYS:HB3	2.54	0.42
1:D:354:SER:HB2	1:D:359:ILE:HG22	2.01	0.42
1:C:254:THR:CG2	2:C:502:PLG:H5A2	2.49	0.42
1:C:278:PRO:CD	1:C:282:LYS:HE3	2.50	0.42
1:C:449:LYS:HB2	1:C:449:LYS:HZ3	1.84	0.42
1:A:107:ASP:HA	1:A:108:PRO:HD2	1.91	0.42
1:B:75:GLU:HB2	1:B:83:TYR:HE2	1.84	0.42
1:D:10:ARG:HB3	1:D:10:ARG:NH2	2.35	0.42
1:C:154:MSE:CE	1:C:169:SER:OG	2.68	0.42
1:A:481:LEU:HB3	1:A:482:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:MSE:HE3	1:D:170:MSE:CE	2.50	0.42
1:B:384:CYS:HB3	1:B:385:ASN:H	1.55	0.41
1:B:384:CYS:SG	1:B:401:LEU:HD22	2.60	0.41
1:A:459:GLN:CA	1:A:462:VAL:HG12	2.45	0.41
1:C:181:ILE:HB	1:C:183:TYR:CE1	2.55	0.41
1:B:107:ASP:OD2	1:B:109:GLN:HB2	2.19	0.41
1:D:183:TYR:CE2	1:D:210:ASP:HB3	2.55	0.41
1:C:39:LYS:HB3	1:D:88:PHE:CE1	2.55	0.41
1:A:372:ARG:HG3	1:A:372:ARG:HH11	1.84	0.41
1:A:137:ARG:NH2	1:C:154:MSE:HE1	2.35	0.41
1:A:462:VAL:CG1	1:A:463:ALA:N	2.84	0.41
1:A:323:GLU:HG2	1:B:17:SER:CB	2.50	0.41
1:B:148:HIS:CE1	1:B:150:THR:HG23	2.51	0.41
1:C:59:ARG:HD3	1:D:23:SER:O	2.19	0.41
1:D:448:PHE:O	1:D:452:LEU:HB2	2.20	0.41
1:B:120:GLY:HA3	2:B:501:PLG:H5A2	2.03	0.41
1:A:319:ALA:HA	1:A:324:PHE:CD2	2.55	0.41
1:D:53:SER:O	1:D:257:LYS:HG2	2.21	0.41
1:D:435:ILE:HD12	1:D:448:PHE:CE1	2.55	0.41
1:D:8:ALA:C	1:D:10:ARG:H	2.23	0.41
1:B:455:ASP:O	1:B:456:GLU:HB2	2.20	0.41
1:B:137:ARG:HA	1:B:168:GLU:O	2.21	0.41
1:A:393:LYS:O	1:A:394:SER:OG	2.30	0.41
1:D:254:THR:HB	1:D:256:HIS:CE1	2.55	0.41
1:A:17:SER:CB	1:B:323:GLU:HG2	2.50	0.41
1:A:297:PHE:CD1	1:A:298:PRO:HA	2.55	0.41
1:D:52:ALA:HA	1:D:404:GLY:HA3	2.02	0.41
1:A:83:TYR:OH	2:B:501:PLG:O	2.36	0.41
1:A:482:PRO:O	1:A:483:ASP:HB3	2.21	0.41
1:A:181:ILE:HD12	1:A:209:LEU:CD2	2.49	0.41
1:C:137:ARG:HA	1:C:168:GLU:O	2.21	0.41
1:D:173:LYS:HE3	1:D:173:LYS:HB3	1.97	0.41
1:D:155:THR:HG22	1:D:158:LYS:H	1.86	0.41
1:B:254:THR:OG1	1:B:257:LYS:HD2	2.21	0.41
1:B:388:THR:HA	1:B:398:PRO:HB3	2.03	0.41
1:B:273:VAL:HG13	1:B:284:THR:O	2.20	0.41
1:D:397:ARG:N	1:D:398:PRO:CD	2.83	0.41
1:C:323:GLU:HG3	1:D:14:LEU:HD13	2.02	0.41
1:A:413:LEU:CD2	1:A:413:LEU:H	2.34	0.41
1:A:121:SER:N	1:A:122:PRO:CD	2.84	0.41
1:B:354:SER:HB2	1:B:359:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:GLY:O	1:D:171:PRO:HA	2.21	0.41
1:B:385:ASN:ND2	1:B:385:ASN:C	2.73	0.41
1:A:46:VAL:HG23	1:A:46:VAL:O	2.21	0.41
1:C:323:GLU:HB3	1:D:18:HIS:HB2	2.02	0.41
1:C:235:LEU:CD2	1:C:328:GLN:HE21	2.33	0.41
1:B:83:TYR:N	1:B:83:TYR:CD2	2.89	0.41
1:C:45:ARG:HG3	1:C:478:LEU:CD2	2.51	0.41
1:C:361:MSE:HE2	1:C:403:LEU:CD1	2.38	0.41
1:C:277:ASP:HB3	1:C:278:PRO:CD	2.42	0.41
1:B:361:MSE:HE3	1:B:401:LEU:CB	2.50	0.41
1:A:361:MSE:O	1:A:400:GLY:CA	2.69	0.41
1:C:46:VAL:HG23	1:C:46:VAL:O	2.19	0.41
1:B:13:THR:HG23	1:B:14:LEU:N	2.36	0.41
1:D:408:LEU:HB3	1:D:413:LEU:HG	2.03	0.41
1:B:215:ARG:CG	1:B:247:HIS:HB3	2.51	0.41
1:D:235:LEU:CD2	1:D:328:GLN:HG3	2.49	0.41
1:A:132:VAL:O	1:A:133:GLU:HB2	2.19	0.41
1:A:148:HIS:CE1	1:A:150:THR:HG23	2.55	0.41
1:A:82:TYR:CE1	1:A:297:PHE:HE2	2.39	0.41
1:B:319:ALA:HA	1:B:324:PHE:CG	2.56	0.41
1:B:436:GLN:O	1:B:437:SER:C	2.59	0.41
1:A:32:GLU:O	1:A:36:ILE:HG13	2.21	0.41
1:C:227:ALA:HB2	1:C:248:CYS:SG	2.61	0.41
1:C:227:ALA:HB3	1:C:251:VAL:HG22	2.02	0.41
1:A:88:PHE:CE1	1:B:39:LYS:HB3	2.56	0.41
1:B:372:ARG:HH12	1:B:397:ARG:HH12	1.67	0.40
1:C:78:PRO:HG2	1:C:93:GLU:HG2	2.03	0.40
1:C:119:SER:C	1:C:122:PRO:HD2	2.42	0.40
1:A:40:GLU:HG3	1:A:44:GLN:HE21	1.85	0.40
1:B:457:LYS:O	1:B:460:SER:HB2	2.21	0.40
1:D:473:ALA:O	1:D:475:ASN:N	2.55	0.40
1:C:153:PHE:CD2	1:C:160:ILE:HB	2.56	0.40
1:D:439:MSE:O	1:D:441:THR:N	2.54	0.40
1:A:408:LEU:HB3	1:A:413:LEU:HG	2.02	0.40
1:C:449:LYS:NZ	1:C:449:LYS:CB	2.83	0.40
1:D:395:ALA:C	1:D:397:ARG:N	2.70	0.40
1:D:235:LEU:CD2	1:D:328:GLN:HE21	2.35	0.40
1:C:356:ASN:HB2	1:C:357:HIS:H	1.66	0.40
1:D:132:VAL:HG12	1:D:136:GLY:HA3	2.04	0.40
1:D:259:LEU:HD12	1:D:259:LEU:HA	1.88	0.40
1:D:158:LYS:HG2	1:D:159:LYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASP:CB	1:A:282:LYS:H	2.32	0.40
1:A:319:ALA:O	1:A:324:PHE:CD2	2.74	0.40
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.89	0.40
1:A:92:LEU:HD11	1:A:310:ALA:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/478 (100%)	401 (84%)	53 (11%)	22 (5%)	3	11
1	B	476/478 (100%)	408 (86%)	53 (11%)	15 (3%)	5	20
1	C	476/478 (100%)	397 (83%)	52 (11%)	27 (6%)	2	6
1	D	476/478 (100%)	405 (85%)	54 (11%)	17 (4%)	4	18
All	All	1904/1912 (100%)	1611 (85%)	212 (11%)	81 (4%)	3	13

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	VAL
1	A	278	PRO
1	A	281	GLY
1	A	393	LYS
1	B	10	ARG
1	B	385	ASN
1	C	12	ALA
1	C	276	VAL
1	C	278	PRO
1	C	385	ASN
1	C	394	SER

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Mol	Chain	Res	Type
1	C	398	PRO
1	C	438	HIS
1	C	440	ALA
1	C	443	ALA
1	C	456	GLU
1	D	440	ALA
1	D	452	LEU
1	A	9	ASP
1	A	10	ARG
1	A	11	ASP
1	A	12	ALA
1	A	398	PRO
1	A	454	GLY
1	A	456	GLU
1	A	474	SER
1	B	395	ALA
1	B	398	PRO
1	B	453	ALA
1	C	75	GLU
1	C	282	LYS
1	C	283	GLU
1	C	455	ASP
1	C	474	SER
1	D	11	ASP
1	D	258	THR
1	D	394	SER
1	D	451	LYS
1	D	474	SER
1	A	75	GLU
1	A	438	HIS
1	A	440	ALA
1	B	15	TRP
1	B	75	GLU
1	B	454	GLY
1	B	456	GLU
1	B	474	SER
1	C	275	SER
1	C	277	ASP
1	C	285	TYR
1	C	399	SER
1	D	75	GLU
1	A	399	SER

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Mol	Chain	Res	Type
1	A	450	GLU
1	B	258	THR
1	B	275	SER
1	B	278	PRO
1	B	438	HIS
1	B	482	PRO
1	C	273	VAL
1	C	281	GLY
1	C	441	THR
1	C	444	THR
1	D	8	ALA
1	D	13	THR
1	D	456	GLU
1	A	103	ALA
1	A	257	LYS
1	A	451	LYS
1	C	103	ALA
1	C	413	LEU
1	D	273	VAL
1	D	275	SER
1	D	413	LEU
1	D	454	GLY
1	D	457	LYS
1	D	482	PRO
1	A	150	THR
1	A	413	LEU
1	C	272	GLY
1	C	482	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	394/383 (103%)	380 (96%)	14 (4%)	42	78
1	B	394/383 (103%)	370 (94%)	24 (6%)	23	56
1	C	394/383 (103%)	370 (94%)	24 (6%)	23	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	394/383 (103%)	373 (95%)	21 (5%)	28	63
All	All	1576/1532 (103%)	1493 (95%)	83 (5%)	28	63

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	MET
1	A	73	TYR
1	A	87	GLU
1	A	113	VAL
1	A	145	ASP
1	A	171	PRO
1	A	213	ARG
1	A	215	ARG
1	A	340	ASP
1	A	342	LEU
1	A	413	LEU
1	A	435	ILE
1	A	445	LEU
1	A	450	GLU
1	B	73	TYR
1	B	87	GLU
1	B	113	VAL
1	B	145	ASP
1	B	171	PRO
1	B	213	ARG
1	B	215	ARG
1	B	231	HIS
1	B	275	SER
1	B	277	ASP
1	B	298	PRO
1	B	340	ASP
1	B	342	LEU
1	B	384	CYS
1	B	385	ASN
1	B	386	LYS
1	B	388	THR
1	B	392	ASP
1	B	393	LYS
1	B	397	ARG
1	B	413	LEU
1	B	435	ILE

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Mol	Chain	Res	Type
1	B	456	GLU
1	B	483	ASP
1	C	73	TYR
1	C	75	GLU
1	C	87	GLU
1	C	113	VAL
1	C	145	ASP
1	C	149	LEU
1	C	156	ASP
1	C	161	SER
1	C	171	PRO
1	C	213	ARG
1	C	215	ARG
1	C	274	ARG
1	C	340	ASP
1	C	342	LEU
1	C	385	ASN
1	C	387	ASN
1	C	392	ASP
1	C	398	PRO
1	C	413	LEU
1	C	435	ILE
1	C	438	HIS
1	C	450	GLU
1	C	483	ASP
1	C	484	PHE
1	D	73	TYR
1	D	87	GLU
1	D	113	VAL
1	D	145	ASP
1	D	155	THR
1	D	156	ASP
1	D	171	PRO
1	D	213	ARG
1	D	215	ARG
1	D	231	HIS
1	D	340	ASP
1	D	342	LEU
1	D	389	CYS
1	D	397	ARG
1	D	413	LEU
1	D	435	ILE

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Mol	Chain	Res	Type
1	D	444	THR
1	D	452	LEU
1	D	456	GLU
1	D	457	LYS
1	D	484	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	71	ASN
1	A	231	HIS
1	A	328	GLN
1	A	471	ASN
1	A	475	ASN
1	B	44	GLN
1	B	70	ASN
1	B	71	ASN
1	B	231	HIS
1	B	328	GLN
1	B	385	ASN
1	B	387	ASN
1	B	471	ASN
1	B	475	ASN
1	C	44	GLN
1	C	70	ASN
1	C	71	ASN
1	C	116	GLN
1	C	194	HIS
1	C	231	HIS
1	C	328	GLN
1	C	385	ASN
1	C	387	ASN
1	C	423	HIS
1	C	471	ASN
1	C	475	ASN
1	D	44	GLN
1	D	70	ASN
1	D	71	ASN
1	D	231	HIS
1	D	247	HIS
1	D	328	GLN

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Mol	Chain	Res	Type
1	D	387	ASN
1	D	471	ASN
1	D	475	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PLG	A	500	-	17,20,20	5.92	10 (58%)	23,28,28	3.36	11 (47%)
3	THF	A	600	-	25,36,36	3.73	13 (52%)	23,50,50	2.34	11 (47%)
2	PLG	B	501	-	17,20,20	6.16	10 (58%)	23,28,28	3.23	9 (39%)
3	THF	B	601	-	25,36,36	3.76	14 (56%)	23,50,50	2.16	9 (39%)
2	PLG	C	502	1	17,20,20	5.16	10 (58%)	23,28,28	3.03	8 (34%)
2	PLG	D	503	1	17,20,20	5.17	11 (64%)	23,28,28	3.01	7 (30%)
3	THF	D	602	-	25,36,36	3.76	15 (60%)	23,50,50	2.21	9 (39%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLG	A	500	-	-	0/10/12/12	0/1/1/1
3	THF	A	600	-	-	0/14/37/37	0/3/3/3
2	PLG	B	501	-	-	0/10/12/12	0/1/1/1
3	THF	B	601	-	-	0/14/37/37	0/3/3/3
2	PLG	C	502	1	-	0/10/12/12	0/1/1/1
2	PLG	D	503	1	-	0/10/12/12	0/1/1/1
3	THF	D	602	-	-	0/14/37/37	0/3/3/3

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PLG	C4A-C4	-15.21	1.34	1.51
2	A	500	PLG	C4A-C4	-14.71	1.35	1.51
3	A	600	THF	C2-N3	-7.97	1.21	1.35
3	B	601	THF	C2-N3	-7.96	1.21	1.35
3	D	602	THF	C2-N3	-7.58	1.21	1.35
2	B	501	PLG	P-OP4	-5.19	1.42	1.60
2	A	500	PLG	P-OP4	-5.15	1.43	1.60
2	C	502	PLG	P-OP4	-4.96	1.43	1.60
2	D	503	PLG	P-OP4	-4.58	1.44	1.60
2	B	501	PLG	P-OP3	-4.16	1.39	1.54
2	C	502	PLG	P-OP3	-4.13	1.39	1.54
2	A	500	PLG	P-OP3	-4.12	1.39	1.54
2	D	503	PLG	P-OP3	-4.10	1.40	1.54
3	A	600	THF	CB-CA	-4.06	1.47	1.53
3	D	602	THF	CB-CA	-3.53	1.48	1.53
3	B	601	THF	CB-CA	-3.33	1.48	1.53
2	A	500	PLG	P-OP2	-3.30	1.42	1.54
2	D	503	PLG	P-OP2	-3.14	1.43	1.54
2	B	501	PLG	P-OP2	-2.92	1.44	1.54
2	C	502	PLG	P-OP2	-2.84	1.44	1.54
2	D	503	PLG	C5A-C5	2.05	1.56	1.50
3	A	600	THF	CA-N	2.12	1.49	1.46
3	D	602	THF	C13-C14	2.18	1.42	1.39
2	A	500	PLG	C6-N1	2.30	1.39	1.34
2	B	501	PLG	C6-N1	2.31	1.39	1.34
2	C	502	PLG	C6-N1	2.35	1.39	1.34
3	B	601	THF	C13-C14	2.42	1.43	1.39
3	B	601	THF	C13-C12	2.44	1.43	1.38
3	D	602	THF	C13-C12	2.45	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	503	PLG	C6-N1	2.52	1.39	1.34
3	D	602	THF	CA-N	2.54	1.50	1.46
3	A	600	THF	C14-N10	2.59	1.46	1.38
3	D	602	THF	C16-C15	2.63	1.43	1.38
2	C	502	PLG	C2-N1	2.76	1.39	1.34
3	D	602	THF	C14-N10	2.76	1.46	1.38
3	A	600	THF	C12-C11	2.91	1.44	1.39
3	B	601	THF	C14-N10	3.03	1.47	1.38
3	D	602	THF	C16-C11	3.05	1.44	1.39
3	A	600	THF	C15-C14	3.05	1.44	1.39
2	A	500	PLG	C2-N1	3.08	1.40	1.34
3	A	600	THF	C16-C15	3.12	1.44	1.38
3	B	601	THF	C16-C15	3.16	1.44	1.38
3	D	602	THF	C15-C14	3.26	1.44	1.39
2	B	501	PLG	C2-N1	3.27	1.41	1.34
3	B	601	THF	C16-C11	3.35	1.45	1.39
3	B	601	THF	C12-C11	3.37	1.45	1.39
3	A	600	THF	C16-C11	3.39	1.45	1.39
2	D	503	PLG	C2-N1	3.40	1.41	1.34
2	C	502	PLG	C4A-C4	3.48	1.55	1.51
3	B	601	THF	C15-C14	3.55	1.45	1.39
2	C	502	PLG	C6-C5	3.57	1.45	1.37
2	A	500	PLG	C6-C5	3.72	1.45	1.37
3	D	602	THF	C12-C11	3.81	1.45	1.39
2	B	501	PLG	C6-C5	3.84	1.46	1.37
2	D	503	PLG	C6-C5	4.03	1.46	1.37
3	A	600	THF	C4-N3	4.07	1.40	1.33
3	B	601	THF	C4-N3	4.10	1.40	1.33
3	D	602	THF	C4-N3	4.37	1.41	1.33
3	D	602	THF	C4A-C8A	4.47	1.46	1.41
2	D	503	PLG	C4A-C4	4.49	1.57	1.51
3	A	600	THF	C4A-C8A	5.35	1.48	1.41
2	B	501	PLG	C5-C4	5.71	1.48	1.40
3	B	601	THF	C4A-C8A	5.86	1.48	1.41
2	C	502	PLG	C5-C4	5.90	1.48	1.40
3	D	602	THF	O4-C4	6.17	1.39	1.24
3	B	601	THF	O4-C4	6.58	1.40	1.24
2	A	500	PLG	C5-C4	6.61	1.49	1.40
3	B	601	THF	C2-NA2	6.69	1.47	1.34
3	D	602	THF	C2-NA2	6.73	1.47	1.34
3	A	600	THF	C2-NA2	6.87	1.48	1.34
3	A	600	THF	O4-C4	6.89	1.41	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	503	PLG	C5-C4	6.99	1.50	1.40
3	B	601	THF	C7-N8	7.69	1.36	1.27
3	A	600	THF	C7-N8	7.93	1.36	1.27
3	D	602	THF	C7-N8	8.87	1.37	1.27
2	C	502	PLG	C3-C4	10.00	1.55	1.40
2	A	500	PLG	C3-C4	10.88	1.56	1.40
2	D	503	PLG	C3-C4	11.02	1.57	1.40
2	B	501	PLG	C3-C4	11.09	1.57	1.40
2	A	500	PLG	C3-C2	11.35	1.48	1.40
2	B	501	PLG	C3-C2	13.00	1.49	1.40
2	D	503	PLG	C3-C2	13.23	1.49	1.40
2	C	502	PLG	C3-C2	15.00	1.51	1.40

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	THF	NA2-C2-N3	-4.17	110.29	117.20
3	B	601	THF	NA2-C2-N3	-4.17	110.29	117.20
3	D	602	THF	NA2-C2-N3	-4.03	110.52	117.20
3	A	600	THF	C13-C14-N10	-3.61	114.14	121.06
3	D	602	THF	C12-C13-C14	-3.17	116.72	120.28
3	B	601	THF	C13-C14-N10	-3.11	115.11	121.06
3	B	601	THF	C12-C13-C14	-2.87	117.06	120.28
2	A	500	PLG	OP3-P-OP1	-2.80	101.58	110.58
3	B	601	THF	C4A-C4-N3	-2.76	119.22	123.46
3	A	600	THF	C12-C13-C14	-2.74	117.20	120.28
3	D	602	THF	C13-C14-N10	-2.74	115.81	121.06
3	A	600	THF	O-C-N	-2.54	117.85	122.44
2	B	501	PLG	OP3-P-OP1	-2.51	102.51	110.58
2	C	502	PLG	OP3-P-OP1	-2.50	102.53	110.58
2	D	503	PLG	OP3-P-OP1	-2.47	102.63	110.58
2	C	502	PLG	C5A-C5-C6	-2.45	114.64	119.28
3	D	602	THF	C4A-C4-N3	-2.44	119.71	123.46
3	A	600	THF	C4A-C4-N3	-2.42	119.73	123.46
2	A	500	PLG	C5A-C5-C6	-2.22	115.07	119.28
2	C	502	PLG	C3-C2-N1	-2.14	117.66	120.61
2	D	503	PLG	C5A-C5-C6	-2.13	115.25	119.28
2	B	501	PLG	C3-C2-N1	-2.01	117.83	120.61
2	A	500	PLG	C5-C6-N1	-2.01	120.38	123.86
3	B	601	THF	C9-N10-C14	2.01	126.53	121.46
3	B	601	THF	C13-C12-C11	2.06	123.16	120.76
3	D	602	THF	C13-C12-C11	2.10	123.19	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	THF	C15-C14-C13	2.11	121.99	119.06
3	A	600	THF	C15-C14-C13	2.13	122.03	119.06
2	D	503	PLG	C5A-C5-C4	2.36	126.44	121.89
3	A	600	THF	C13-C12-C11	2.40	123.54	120.76
2	C	502	PLG	C5A-C5-C4	2.45	126.61	121.89
3	B	601	THF	C8A-N8-C7	2.46	123.80	116.52
2	A	500	PLG	C5A-C5-C4	2.48	126.67	121.89
3	A	600	THF	C9-N10-C14	2.57	127.95	121.46
3	A	600	THF	C8A-N8-C7	2.74	124.61	116.52
3	D	602	THF	C11-C-N	2.76	121.84	116.93
3	B	601	THF	C11-C-N	2.87	122.04	116.93
2	B	501	PLG	C-CA-N	3.38	117.43	111.66
2	C	502	PLG	C6-N1-C2	3.56	126.55	119.28
2	D	503	PLG	C6-N1-C2	3.64	126.70	119.28
2	B	501	PLG	C6-N1-C2	3.67	126.77	119.28
3	D	602	THF	C8A-N8-C7	3.69	127.43	116.52
3	A	600	THF	C11-C-N	3.73	123.57	116.93
2	A	500	PLG	C6-N1-C2	3.77	126.97	119.28
2	A	500	PLG	O3-C3-C2	3.89	124.43	117.66
2	B	501	PLG	C4-C4A-N	3.96	118.43	111.66
2	B	501	PLG	O3-C3-C2	4.01	124.63	117.66
2	D	503	PLG	O3-C3-C2	4.05	124.70	117.66
2	A	500	PLG	C-CA-N	4.43	119.22	111.66
2	A	500	PLG	C4-C4A-N	4.66	119.61	111.66
2	C	502	PLG	O3-C3-C2	4.73	125.88	117.66
3	B	601	THF	N3-C2-N1	4.82	133.44	125.53
3	A	600	THF	N3-C2-N1	4.89	133.56	125.53
3	D	602	THF	N3-C2-N1	4.98	133.69	125.53
2	A	500	PLG	CA-N-C4A	5.54	123.39	112.03
2	B	501	PLG	CA-N-C4A	5.97	124.25	112.03
2	D	503	PLG	OP3-P-OP4	7.47	128.07	106.56
2	B	501	PLG	OP3-P-OP4	7.56	128.32	106.56
2	B	501	PLG	OP4-C5A-C5	7.69	121.71	108.99
2	C	502	PLG	OP3-P-OP4	7.70	128.74	106.56
2	A	500	PLG	OP4-C5A-C5	7.88	122.02	108.99
2	A	500	PLG	OP3-P-OP4	7.94	129.43	106.56
2	C	502	PLG	OP4-C5A-C5	8.89	123.69	108.99
2	D	503	PLG	OP4-C5A-C5	9.59	124.85	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	PLG	1	0
3	A	600	THF	3	0
2	B	501	PLG	5	0
3	B	601	THF	1	0
2	C	502	PLG	3	0
2	D	503	PLG	2	0
3	D	602	THF	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	467/478 (97%)	0.44	42 (8%) 12 7	44, 79, 140, 151	0
1	B	467/478 (97%)	0.24	26 (5%) 28 21	42, 68, 139, 151	0
1	C	467/478 (97%)	0.30	31 (6%) 22 16	44, 79, 133, 151	0
1	D	467/478 (97%)	0.37	36 (7%) 16 11	44, 81, 138, 151	0
All	All	1868/1912 (97%)	0.34	135 (7%) 18 12	42, 76, 139, 151	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9	ASP	9.7
1	D	484	PHE	9.1
1	C	8	ALA	7.3
1	D	483	ASP	6.9
1	A	8	ALA	6.5
1	B	280	THR	6.2
1	C	484	PHE	6.1
1	D	281	GLY	6.0
1	B	9	ASP	5.9
1	C	11	ASP	5.9
1	D	8	ALA	5.9
1	D	7	MET	5.7
1	D	11	ASP	5.5
1	D	9	ASP	5.5
1	B	7	MET	5.4
1	D	10	ARG	5.3
1	A	7	MET	5.3
1	C	282	LYS	5.3
1	C	7	MET	5.3
1	C	10	ARG	5.1
1	B	8	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	454	GLY	5.0
1	C	276	VAL	5.0
1	A	484	PHE	5.0
1	D	280	THR	4.9
1	D	276	VAL	4.9
1	C	283	GLU	4.7
1	C	278	PRO	4.5
1	A	280	THR	4.5
1	B	14	LEU	4.5
1	C	277	ASP	4.5
1	A	365	SER	4.3
1	A	278	PRO	4.3
1	D	282	LYS	4.3
1	A	362	ASP	4.3
1	D	14	LEU	4.3
1	D	396	LEU	4.3
1	A	392	ASP	4.2
1	C	281	GLY	4.2
1	A	277	ASP	4.2
1	D	278	PRO	4.1
1	A	10	ARG	4.1
1	B	10	ARG	4.0
1	A	276	VAL	4.0
1	B	11	ASP	4.0
1	A	455	ASP	3.9
1	D	279	LYS	3.8
1	B	484	PHE	3.8
1	C	275	SER	3.7
1	B	277	ASP	3.7
1	A	437	SER	3.7
1	C	284	THR	3.7
1	C	482	PRO	3.7
1	A	9	ASP	3.7
1	B	281	GLY	3.6
1	B	455	ASP	3.5
1	A	368	THR	3.5
1	D	284	THR	3.4
1	D	455	ASP	3.4
1	A	454	GLY	3.4
1	D	13	THR	3.4
1	C	280	THR	3.3
1	A	279	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	285	TYR	3.2
1	B	396	LEU	3.2
1	D	277	ASP	3.2
1	B	278	PRO	3.1
1	D	440	ALA	3.1
1	B	276	VAL	3.1
1	B	275	SER	3.1
1	D	454	GLY	3.0
1	D	12	ALA	3.0
1	A	458	ILE	2.9
1	A	444	THR	2.9
1	A	384	CYS	2.9
1	D	275	SER	2.9
1	B	285	TYR	2.9
1	A	438	HIS	2.9
1	A	275	SER	2.8
1	B	284	THR	2.8
1	A	451	LYS	2.8
1	C	279	LYS	2.8
1	B	393	LYS	2.8
1	D	407	ALA	2.7
1	D	53	SER	2.7
1	D	457	LYS	2.7
1	A	285	TYR	2.7
1	D	459	GLN	2.6
1	D	285	TYR	2.6
1	C	407	ALA	2.6
1	C	273	VAL	2.5
1	A	202	THR	2.5
1	D	283	GLU	2.5
1	B	228	ASP	2.5
1	A	483	ASP	2.5
1	C	396	LEU	2.4
1	A	453	ALA	2.4
1	C	28	ASP	2.4
1	A	347	TYR	2.4
1	B	482	PRO	2.4
1	C	231	HIS	2.4
1	D	261	GLY	2.4
1	D	202	THR	2.4
1	A	465	LEU	2.4
1	C	12	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	16	ALA	2.3
1	C	483	ASP	2.3
1	A	284	THR	2.3
1	A	385	ASN	2.3
1	A	370	GLY	2.3
1	B	483	ASP	2.2
1	C	435	ILE	2.2
1	A	457	LYS	2.2
1	C	71	ASN	2.2
1	B	157	LYS	2.2
1	A	175	TYR	2.2
1	B	392	ASP	2.2
1	C	52	ALA	2.2
1	C	393	LYS	2.1
1	A	273	VAL	2.1
1	A	256	HIS	2.1
1	B	256	HIS	2.1
1	A	12	ALA	2.1
1	A	230	ALA	2.1
1	D	443	ALA	2.1
1	A	51	ILE	2.1
1	A	364	ARG	2.1
1	D	460	SER	2.1
1	C	456	GLU	2.0
1	A	433	LEU	2.0
1	B	15	TRP	2.0
1	C	367	GLY	2.0
1	D	255	THR	2.0
1	D	463	ALA	2.0
1	A	233	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	THF	D	602	34/34	0.53	0.70	7.62	151,151,151,151	0
3	THF	B	601	34/34	0.75	0.34	2.31	132,132,132,132	0
3	THF	A	600	34/34	0.85	0.29	0.98	106,106,106,106	0
2	PLG	D	503	20/20	0.94	0.29	0.64	88,88,118,118	0
2	PLG	B	501	20/20	0.97	0.28	0.60	79,79,88,88	0
2	PLG	C	502	20/20	0.94	0.25	0.35	77,77,112,112	0
2	PLG	A	500	20/20	0.97	0.21	-0.52	70,70,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.