



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:02 PM GMT

PDB ID : 3SL5
Title : Crystal structure of the catalytic domain of PDE4D2 complexed with compound 10d
Authors : Feil, S.F.
Deposited on : 2011-06-24
Resolution : 2.65 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

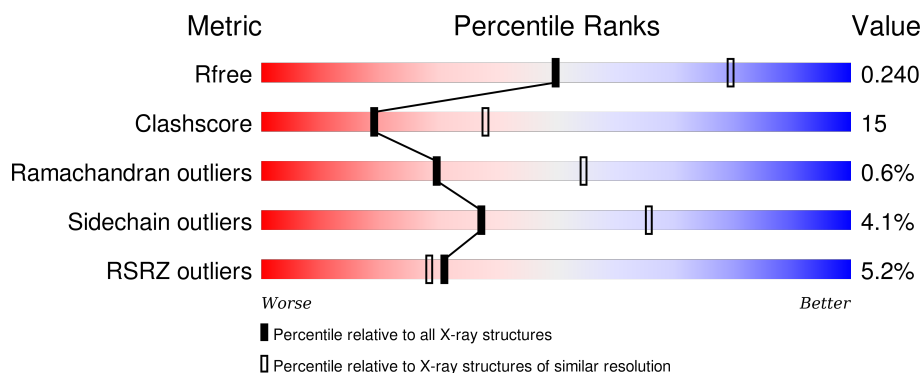
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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))
R_{free}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	359	<div> <div>6%</div> <div>65%</div> <div>23%</div> <div>9%</div> </div>
1	B	359	<div> <div>3%</div> <div>55%</div> <div>32%</div> <div>9%</div> </div>
1	C	359	<div> <div>6%</div> <div>61%</div> <div>27%</div> <div>9%</div> </div>
1	D	359	<div> <div>4%</div> <div>67%</div> <div>20%</div> <div>10%</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	J25	A	1	-	-	X	X
3	J25	B	1	-	-	-	X
4	EDO	B	2	-	-	-	X
4	EDO	C	3	-	-	-	X
4	EDO	C	6	-	-	-	X
4	EDO	D	2	-	-	-	X
4	EDO	D	3	-	-	X	-
4	EDO	D	7	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11156 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.

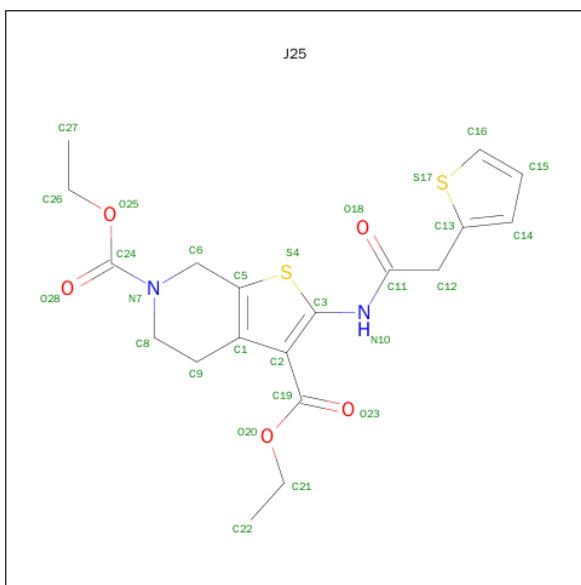
- Molecule 1 is a protein called cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2651	1676	453	508	14			
1	B	325	Total	C	N	O	S	0	0	0
			2631	1664	450	503	14			
1	C	325	Total	C	N	O	S	0	0	0
			2631	1663	449	505	14			
1	D	324	Total	C	N	O	S	0	0	0
			2622	1659	448	501	14			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is DIETHYL 2-[(THIOPHEN-2-YLACETYL)AMINO]-4,7-DIHYDROTHIENO[2,3-C]PYRIDINE-3,6(5H)-DICARBOXYLATE (three-letter code: J25) (formula: C₁₉H₂₂N₂O₅S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			28	19	2	5	2		
3	B	1	Total	C	N	O	S	0	0
			28	19	2	5	2		
3	C	1	Total	C	N	O	S	0	0
			28	19	2	5	2		
3	D	1	Total	C	N	O	S	0	0
			28	19	2	5	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



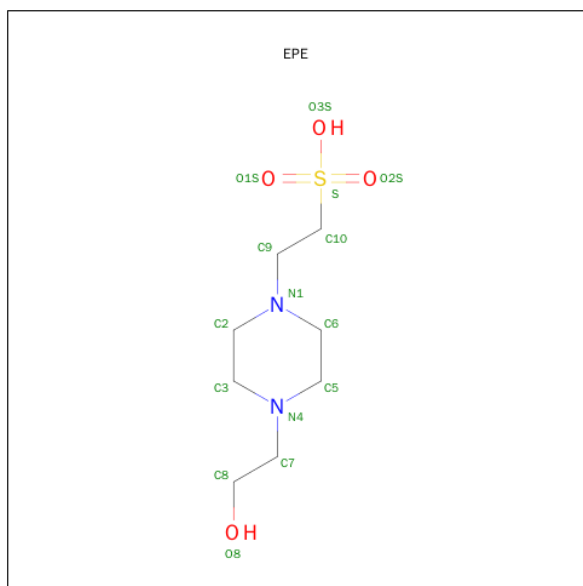
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

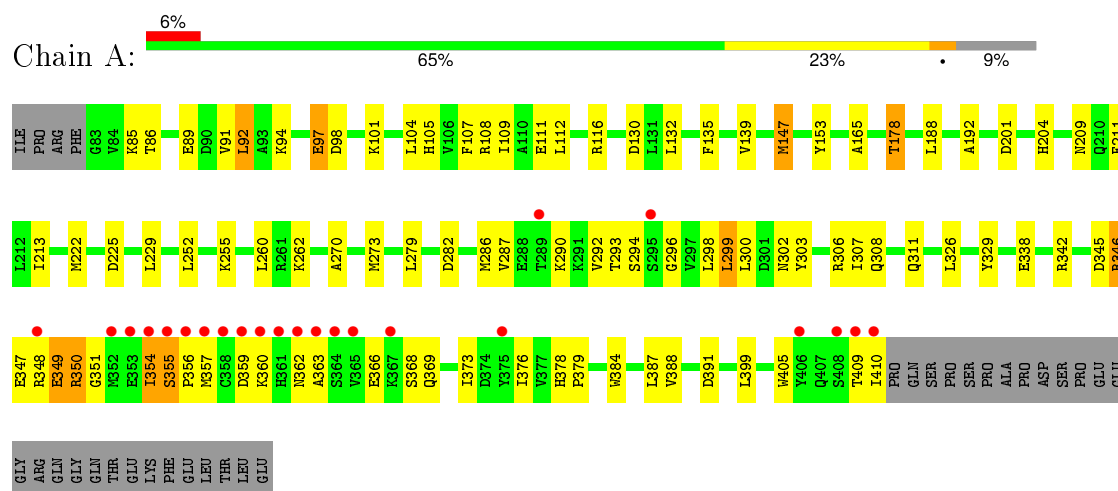
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	107	Total 107	O 107	0	0
7	B	92	Total 92	O 92	0	0
7	C	82	Total 82	O 82	0	0
7	D	133	Total 133	O 133	0	0

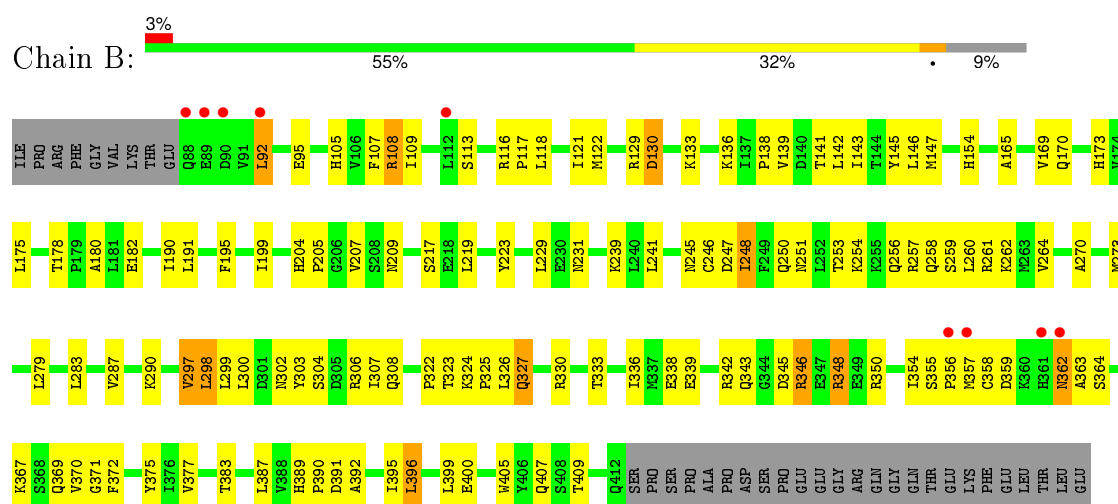
3 Residue-property plots

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.

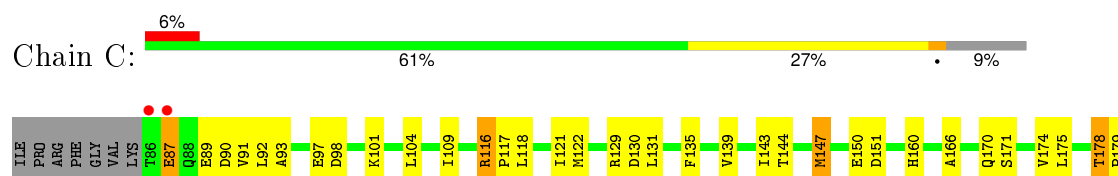
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

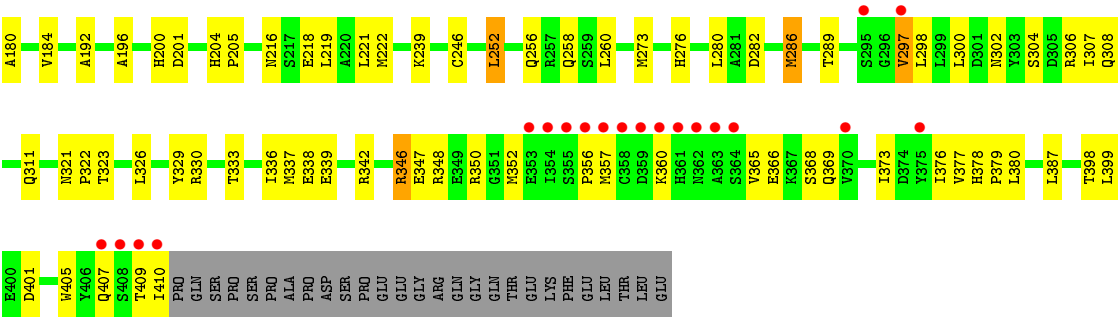


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D





• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.39Å 109.97Å 159.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.73 – 2.65 61.73 – 2.65	Depositor EDS
% Data completeness (in resolution range)	91.3 (61.73-2.65) 91.3 (61.73-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.171 , 0.242 0.170 , 0.240	Depositor DCC
R_{free} test set	2365 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 46142 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11156	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, ZN, DMS, EDO, J25

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	0.39	0/2704	0.52	0/3672
1	B	0.37	0/2685	0.53	0/3648
1	C	0.38	0/2684	0.53	0/3646
1	D	0.42	0/2676	0.54	0/3636
All	All	0.39	0/10749	0.53	0/14602

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2651	0	2609	85	0
1	B	2631	0	2586	104	0
1	C	2631	0	2584	77	0
1	D	2622	0	2578	60	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	28	0	22	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	22	7	0
3	C	28	0	22	6	0
3	D	28	0	22	4	0
4	A	8	0	12	1	0
4	B	8	0	12	3	0
4	C	20	0	30	2	0
4	D	32	0	48	6	0
5	A	4	0	6	0	0
6	C	15	0	17	0	0
7	A	107	0	0	5	0
7	B	92	0	0	7	0
7	C	82	0	0	3	0
7	D	133	0	0	3	0
All	All	11156	0	10570	324	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 15.

All (324) 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:A:368:SER:HB3	3:A:1:J25:H22	1.40	1.00
1:C:368:SER:HB3	3:C:1:J25:H22	1.47	0.95
1:B:348:ARG:HG3	1:B:354:ILE:HD11	1.55	0.86
1:B:108:ARG:HH11	1:B:108:ARG:HG3	1.37	0.86
1:D:273:MET:HG3	3:D:1:J25:H6	1.55	0.86
1:D:304:SER:O	1:D:308:GLN:HG3	1.75	0.85
1:A:273:MET:HG3	3:A:1:J25:H6	1.58	0.85
3:A:1:J25:H6A	3:A:1:J25:H26	1.58	0.85
1:B:108:ARG:CG	1:B:108:ARG:HH11	1.90	0.84
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.43	0.83
1:A:86:THR:OG1	1:A:89:GLU:HG3	1.79	0.83
1:B:182:GLU:O	1:B:297:VAL:HG21	1.77	0.82
1:A:116:ARG:HE	1:A:147:MET:HE2	1.43	0.81
3:B:1:J25:H8	3:B:1:J25:H26A	1.63	0.79
1:C:135:PHE:HA	4:C:2:EDO:H21	1.62	0.79
1:D:190:ILE:HD11	4:D:3:EDO:H21	1.63	0.79
1:D:88:GLN:HB3	1:D:91:VAL:HG23	1.67	0.77
1:B:105:HIS:CE1	1:B:107:PHE:HB2	2.19	0.77
1:A:338:GLU:O	1:A:342:ARG:HG3	1.87	0.75
1:D:185:PHE:H	4:D:3:EDO:H11	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ARG:HG2	1:C:147:MET:HE1	1.70	0.73
1:A:132:LEU:HD22	1:A:139:VAL:HG12	1.70	0.72
1:C:337:MET:HG3	1:C:365:VAL:HG22	1.72	0.72
1:B:253:THR:HG23	1:B:256:GLN:OE1	1.91	0.71
1:B:254:LYS:O	1:B:258:GLN:HG3	1.90	0.71
1:D:326:LEU:O	1:D:330:ARG:HG3	1.90	0.71
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.74	0.69
1:C:180:ALA:O	1:C:297:VAL:HG22	1.93	0.69
1:A:366:GLU:HG2	1:A:409:THR:CG2	2.22	0.69
1:C:347:GLU:HG2	1:C:352:MET:HE2	1.74	0.68
1:A:369:GLN:O	1:A:373:ILE:HG13	1.94	0.68
1:A:292:VAL:CG1	1:A:296:GLY:HA2	2.24	0.68
1:B:217:SER:HB2	7:D:527:HOH:O	1.94	0.67
3:B:1:J25:C8	3:B:1:J25:H26A	2.25	0.66
1:A:104:LEU:HD11	1:A:109:ILE:HD11	1.78	0.66
1:A:287:VAL:O	1:A:290:LYS:HB2	1.96	0.66
1:B:109:ILE:O	1:B:113:SER:HB2	1.96	0.65
1:A:354:ILE:HG21	1:A:359:ASP:HA	1.79	0.65
1:D:348:ARG:HB3	1:D:354:ILE:HD11	1.78	0.65
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.79	0.64
1:A:369:GLN:NE2	3:A:1:J25:H21	2.13	0.64
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.33	0.64
1:C:273:MET:HE2	3:C:1:J25:O28	1.98	0.63
1:D:322:PRO:HG3	3:D:1:J25:H15	1.79	0.63
1:D:88:GLN:HG3	1:D:90:ASP:H	1.62	0.63
1:A:105:HIS:CD2	1:A:108:ARG:H	2.16	0.63
1:C:348:ARG:HH22	1:C:360:LYS:HE2	1.62	0.63
1:C:139:VAL:HG23	7:C:547:HOH:O	1.97	0.63
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.81	0.62
1:B:364:SER:HB2	7:B:529:HOH:O	1.99	0.62
1:A:302:ASN:O	1:A:306:ARG:HG3	1.99	0.62
1:B:372:PHE:HE2	3:B:1:J25:H14	1.64	0.62
1:B:298:LEU:HD11	1:B:387:LEU:HD11	1.81	0.62
1:A:345:ASP:O	1:A:349:GLU:HG3	1.99	0.62
1:A:116:ARG:HE	1:A:147:MET:CE	2.11	0.62
1:A:359:ASP:CG	1:A:362:ASN:HB2	2.20	0.62
1:B:108:ARG:NH1	1:B:108:ARG:HG3	2.13	0.61
1:A:292:VAL:HG12	1:A:293:THR:N	2.15	0.61
1:B:141:THR:HG22	1:B:248:ILE:HG22	1.82	0.61
1:C:302:ASN:HD22	1:C:304:SER:HB3	1.64	0.61
1:B:302:ASN:O	1:B:306:ARG:HG3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:NH1	1:A:108:ARG:HG2	2.16	0.60
1:C:116:ARG:CG	1:C:147:MET:HE1	2.31	0.60
1:A:366:GLU:HG2	1:A:409:THR:HB	1.83	0.60
1:C:369:GLN:O	1:C:373:ILE:HG13	2.02	0.59
1:B:129:ARG:HH12	1:B:190:ILE:HD13	1.66	0.59
1:D:270:ALA:HB1	1:D:279:LEU:HD11	1.85	0.59
1:C:184:VAL:HG11	1:C:300:LEU:HD12	1.85	0.59
1:B:396:LEU:O	1:B:400:GLU:HG3	2.03	0.59
1:A:85:LYS:HB3	1:A:89:GLU:HB2	1.84	0.58
1:B:372:PHE:CE2	3:B:1:J25:H14	2.38	0.58
1:C:87:GLU:O	1:C:91:VAL:HG23	2.03	0.58
1:D:223:TYR:CE1	1:D:231:ASN:HB3	2.39	0.57
1:A:369:GLN:HE22	3:A:1:J25:H21	1.69	0.57
1:B:338:GLU:OE2	1:B:342:ARG:NH2	2.37	0.57
1:D:94:LYS:O	1:D:97:GLU:HB2	2.05	0.57
1:C:282:ASP:HB3	1:C:308:GLN:NE2	2.20	0.57
1:A:105:HIS:HD2	1:A:108:ARG:H	1.52	0.57
1:B:355:SER:HB2	1:B:358:CYS:SG	2.45	0.57
1:C:222:MET:HG2	1:D:222:MET:CE	2.35	0.57
1:D:356:PRO:O	1:D:357:MET:HE2	2.05	0.57
1:D:96:LEU:HD11	1:D:120:VAL:HG13	1.87	0.57
1:A:225:ASP:OD1	1:B:261:ARG:NH2	2.38	0.57
1:D:192:ALA:HB2	1:D:260:LEU:HD12	1.87	0.56
3:A:1:J25:C6	3:A:1:J25:H26	2.34	0.56
1:C:304:SER:O	1:C:308:GLN:HB2	2.05	0.56
1:A:307:ILE:O	1:A:311:GLN:HG3	2.04	0.56
1:C:116:ARG:N	1:C:117:PRO:CD	2.68	0.56
1:C:160:HIS:ND1	1:C:339:GLU:OE2	2.31	0.56
1:D:219:LEU:HD21	1:D:232:HIS:CD2	2.41	0.56
1:C:121:ILE:HD12	1:C:166:ALA:HB1	1.88	0.56
1:D:355:SER:HB2	1:D:358:CYS:SG	2.45	0.56
1:C:129:ARG:HB2	1:C:131:LEU:HG	1.88	0.56
1:D:105:HIS:CE1	1:D:107:PHE:HB2	2.41	0.56
1:A:366:GLU:HG2	1:A:409:THR:HG21	1.88	0.55
1:B:326:LEU:HD21	1:B:405:TRP:CE2	2.41	0.55
1:B:116:ARG:N	1:B:117:PRO:CD	2.69	0.55
1:D:346:ARG:O	1:D:350:ARG:HG3	2.06	0.55
1:C:216:ASN:HB3	7:D:587:HOH:O	2.06	0.55
1:A:292:VAL:HG11	1:A:296:GLY:HA2	1.88	0.55
1:B:261:ARG:NH1	7:B:534:HOH:O	2.39	0.54
1:A:342:ARG:HD3	7:A:606:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLN:OE1	3:A:1:J25:H15	2.08	0.54
1:A:366:GLU:HG2	1:A:409:THR:CB	2.38	0.54
1:C:192:ALA:HB2	1:C:260:LEU:HD12	1.89	0.54
1:B:105:HIS:HE1	1:B:107:PHE:HB2	1.73	0.54
1:A:116:ARG:HG3	1:A:147:MET:HE3	1.90	0.53
1:B:92:LEU:HD22	1:B:92:LEU:O	2.07	0.53
1:C:398:THR:O	1:C:401:ASP:HB2	2.09	0.53
1:B:223:TYR:CE1	1:B:231:ASN:HB3	2.43	0.53
1:B:364:SER:OG	1:B:367:LYS:HB2	2.09	0.53
1:A:92:LEU:O	1:A:92:LEU:HD22	2.08	0.53
1:D:213:ILE:HD13	1:D:225:ASP:HB3	1.91	0.53
1:D:178:THR:OG1	4:D:6:EDO:H22	2.09	0.53
1:A:188:LEU:HD23	4:A:4:EDO:H21	1.90	0.52
1:A:298:LEU:HD21	1:A:387:LEU:O	2.10	0.52
1:C:171:SER:O	1:C:175:LEU:HG	2.09	0.52
1:C:376:ILE:CD1	3:C:1:J25:H26A	2.40	0.52
1:B:355:SER:HB3	1:B:356:PRO:HD2	1.92	0.52
1:A:349:GLU:C	1:A:351:GLY:H	2.13	0.51
1:D:176:LEU:HD13	1:D:190:ILE:HG23	1.92	0.51
1:C:298:LEU:HD11	1:C:387:LEU:HD11	1.93	0.51
1:A:357:MET:SD	3:A:1:J25:H22A	2.50	0.51
1:C:356:PRO:O	1:C:357:MET:HB2	2.10	0.51
1:C:326:LEU:HD21	1:C:405:TRP:CE2	2.45	0.51
1:B:304:SER:O	1:B:308:GLN:HG3	2.10	0.51
1:B:354:ILE:HG21	1:B:359:ASP:HB2	1.91	0.51
1:C:218:GLU:O	1:C:222:MET:HB2	2.11	0.51
1:C:196:ALA:O	1:C:200:HIS:HB3	2.10	0.51
1:A:209:ASN:O	1:A:213:ILE:HG13	2.10	0.51
1:C:302:ASN:ND2	1:C:304:SER:HB3	2.25	0.51
1:B:118:LEU:O	1:B:122:MET:HB2	2.11	0.51
1:C:116:ARG:NH2	1:C:151:ASP:OD2	2.43	0.51
1:B:143:ILE:O	1:B:147:MET:HG2	2.11	0.51
1:C:323:THR:HG22	1:C:399:LEU:HD13	1.92	0.51
1:A:384:TRP:O	1:A:388:VAL:HG22	2.11	0.50
1:B:389:HIS:CD2	1:B:390:PRO:HA	2.46	0.50
1:B:142:LEU:O	1:B:146:LEU:HG	2.11	0.50
1:A:282:ASP:HB3	1:A:308:GLN:OE1	2.11	0.50
1:C:93:ALA:O	1:C:97:GLU:HG3	2.12	0.50
1:C:346:ARG:O	1:C:350:ARG:HG3	2.12	0.50
1:B:239:LYS:HE2	1:D:218:GLU:CG	2.42	0.50
1:B:239:LYS:HE2	1:D:218:GLU:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:GLN:NE2	1:C:410:ILE:HD12	2.27	0.49
1:D:90:ASP:O	1:D:94:LYS:HD3	2.11	0.49
1:A:132:LEU:CD2	1:A:139:VAL:HG12	2.42	0.49
1:C:116:ARG:NH1	1:C:150:GLU:HG2	2.28	0.49
1:B:138:PRO:HG2	1:B:250:GLN:OE1	2.12	0.49
1:D:239:LYS:HE3	1:D:242:GLN:OE1	2.12	0.49
1:A:91:VAL:HG12	1:A:112:LEU:HD13	1.95	0.49
1:A:359:ASP:O	1:A:363:ALA:HB2	2.13	0.49
1:B:260:LEU:O	1:B:264:VAL:HG23	2.12	0.49
1:B:129:ARG:HE	1:B:173:HIS:CE1	2.31	0.49
1:C:366:GLU:CD	1:C:366:GLU:H	2.15	0.49
1:A:201:ASP:O	1:A:204:HIS:HB2	2.12	0.49
1:C:273:MET:HG3	3:C:1:J25:H6	1.94	0.48
1:B:273:MET:HG3	3:B:1:J25:H6	1.94	0.48
1:D:209:ASN:O	1:D:213:ILE:HG13	2.13	0.48
1:B:283:LEU:O	1:B:287:VAL:HG23	2.13	0.48
3:B:1:J25:S4	3:B:1:J25:O18	2.71	0.48
1:B:342:ARG:O	1:B:346:ARG:HG3	2.13	0.48
1:D:216:ASN:HD21	1:D:221:LEU:HD21	1.78	0.48
1:B:345:ASP:OD1	1:B:348:ARG:NH2	2.45	0.48
1:B:409:THR:HG22	1:B:409:THR:O	2.13	0.48
1:D:393:GLN:HG2	7:D:613:HOH:O	2.12	0.48
1:D:342:ARG:HD2	1:D:342:ARG:HA	1.60	0.48
1:A:409:THR:O	1:A:410:ILE:HG22	2.14	0.48
1:C:302:ASN:O	1:C:306:ARG:HG3	2.13	0.48
1:B:136:LYS:HB2	1:B:251:ASN:HB2	1.95	0.48
1:D:223:TYR:CD1	1:D:231:ASN:HB3	2.48	0.48
1:C:201:ASP:O	1:C:204:HIS:HB2	2.13	0.48
1:B:116:ARG:HD2	1:B:147:MET:SD	2.54	0.48
1:B:136:LYS:O	1:B:138:PRO:HD3	2.13	0.48
1:B:290:LYS:HD3	7:B:556:HOH:O	2.14	0.48
1:A:108:ARG:HH11	1:A:108:ARG:CG	2.22	0.48
1:B:362:ASN:ND2	1:B:362:ASN:H	2.12	0.48
1:C:118:LEU:O	1:C:122:MET:HB2	2.15	0.47
1:B:333:THR:HA	1:B:336:ILE:HG22	1.96	0.47
1:B:257:ARG:HD3	7:B:536:HOH:O	2.14	0.47
1:A:94:LYS:O	1:A:97:GLU:HB2	2.13	0.47
1:B:339:GLU:HG2	4:B:3:EDO:H21	1.96	0.47
1:A:346:ARG:O	1:A:350:ARG:HG3	2.15	0.47
1:B:121:ILE:HG21	1:B:170:GLN:HB2	1.97	0.47
1:D:252:LEU:HB2	1:D:257:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ARG:HD3	1:C:405:TRP:CZ3	2.49	0.47
1:C:333:THR:HA	1:C:336:ILE:HG22	1.96	0.47
1:B:209:ASN:HB3	7:B:589:HOH:O	2.15	0.47
1:D:252:LEU:N	1:D:252:LEU:HD23	2.30	0.47
1:D:108:ARG:HH21	1:D:112:LEU:HD21	1.80	0.47
1:C:116:ARG:HH22	1:C:151:ASP:CG	2.17	0.47
1:D:330:ARG:HD2	1:D:405:TRP:CZ3	2.49	0.47
1:B:333:THR:O	1:B:336:ILE:HG22	2.15	0.46
1:D:142:LEU:O	1:D:146:LEU:HG	2.15	0.46
1:D:302:ASN:O	1:D:306:ARG:HG3	2.15	0.46
1:B:246:CYS:O	1:B:248:ILE:HG23	2.14	0.46
1:B:165:ALA:O	1:B:169:VAL:HG23	2.15	0.46
1:C:321:ASN:OD1	3:C:1:J25:H12	2.15	0.46
1:B:195:PHE:CE2	1:B:199:ILE:HD13	2.51	0.46
1:A:292:VAL:CG1	1:A:293:THR:N	2.78	0.46
1:D:321:ASN:CB	1:D:322:PRO:HD3	2.43	0.46
1:C:184:VAL:CG1	1:C:300:LEU:HD12	2.45	0.46
1:B:191:LEU:HD23	1:B:260:LEU:CD1	2.45	0.46
1:D:369:GLN:O	1:D:373:ILE:HG13	2.15	0.46
1:A:153:TYR:CZ	1:A:165:ALA:HB2	2.51	0.46
1:B:327:GLN:NE2	1:B:327:GLN:HA	2.31	0.46
1:A:104:LEU:HD21	1:A:109:ILE:HD12	1.97	0.45
1:B:245:ASN:ND2	7:B:532:HOH:O	2.49	0.45
1:C:143:ILE:O	1:C:147:MET:HG2	2.16	0.45
1:B:130:ASP:OD2	1:B:133:LYS:HB2	2.16	0.45
1:A:178:THR:OG1	1:A:391:ASP:HB3	2.17	0.45
1:D:307:ILE:O	1:D:311:GLN:HG3	2.17	0.45
1:A:345:ASP:O	1:A:348:ARG:HG2	2.17	0.45
1:B:348:ARG:HH11	1:B:354:ILE:HD11	1.81	0.45
1:B:346:ARG:NH1	1:D:151:ASP:OD1	2.50	0.45
1:D:299:LEU:HD13	1:D:299:LEU:C	2.37	0.45
1:C:130:ASP:HA	7:C:516:HOH:O	2.17	0.45
1:C:239:LYS:HG3	7:C:575:HOH:O	2.17	0.45
1:B:129:ARG:NH1	1:B:190:ILE:HD13	2.31	0.45
1:B:204:HIS:HA	1:B:205:PRO:HD3	1.86	0.45
1:C:98:ASP:HA	1:C:101:LYS:NZ	2.31	0.45
1:B:327:GLN:NE2	7:B:548:HOH:O	2.38	0.44
1:C:170:GLN:O	1:C:174:VAL:HG23	2.17	0.44
1:D:185:PHE:H	4:D:3:EDO:C1	2.28	0.44
1:D:349:GLU:C	1:D:351:GLY:H	2.21	0.44
1:B:241:LEU:HD22	1:B:247:ASP:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:GLY:O	1:B:375:TYR:HD1	1.99	0.44
1:A:255:LYS:HA	7:A:542:HOH:O	2.16	0.44
1:B:298:LEU:HD23	1:B:298:LEU:HA	1.87	0.44
1:B:247:ASP:O	1:B:248:ILE:HG12	2.16	0.44
1:A:368:SER:HB3	3:A:1:J25:C22	2.28	0.44
1:D:249:PHE:CZ	1:D:260:LEU:HD21	2.53	0.44
1:A:135:PHE:HB3	1:A:252:LEU:HD11	2.00	0.44
1:B:191:LEU:HD23	1:B:260:LEU:HD13	1.99	0.44
1:C:366:GLU:HG2	1:C:409:THR:CG2	2.48	0.44
1:C:221:LEU:C	1:C:221:LEU:HD13	2.38	0.44
1:A:107:PHE:O	1:A:111:GLU:HG3	2.18	0.44
1:A:262:LYS:HE3	7:A:563:HOH:O	2.18	0.44
1:A:378:HIS:HA	1:A:399:LEU:HD21	2.00	0.43
1:A:355:SER:HB3	1:A:356:PRO:CD	2.48	0.43
1:D:183:ALA:N	4:D:3:EDO:H12	2.33	0.43
1:C:329:TYR:HE1	3:C:1:J25:H15	1.83	0.43
1:D:357:MET:HE1	3:D:1:J25:H9	2.00	0.43
1:D:103:GLY:O	1:D:104:LEU:C	2.55	0.43
1:A:299:LEU:HD22	1:A:300:LEU:N	2.34	0.43
1:A:192:ALA:HB2	1:A:260:LEU:HD12	2.01	0.43
1:A:356:PRO:O	1:A:357:MET:HB2	2.19	0.43
1:B:348:ARG:HH11	1:B:354:ILE:CD1	2.32	0.43
1:A:354:ILE:H	1:A:354:ILE:HG13	1.62	0.43
1:B:300:LEU:O	1:B:306:ARG:NH1	2.50	0.43
1:B:355:SER:HB3	1:B:356:PRO:CD	2.49	0.43
1:B:342:ARG:O	1:B:346:ARG:CG	2.67	0.43
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.83	0.43
1:A:225:ASP:CG	1:B:261:ARG:NH2	2.72	0.43
1:A:303:TYR:O	1:A:307:ILE:HG22	2.19	0.43
1:C:144:THR:HG22	1:C:246:CYS:SG	2.58	0.43
1:A:329:TYR:HE1	3:A:1:J25:H15	1.84	0.43
1:B:369:GLN:OE1	3:B:1:J25:H15	2.19	0.43
1:B:324:LYS:O	1:B:325:PRO:C	2.57	0.43
1:A:342:ARG:HB3	7:A:606:HOH:O	2.18	0.42
1:A:360:LYS:C	1:A:362:ASN:H	2.22	0.42
1:C:104:LEU:HD11	1:C:109:ILE:HD11	2.01	0.42
1:A:349:GLU:HG3	1:A:349:GLU:H	1.49	0.42
1:D:152:HIS:CE1	4:D:2:EDO:H11	2.55	0.42
1:B:339:GLU:OE2	4:B:3:EDO:H21	2.20	0.42
1:B:392:ALA:O	1:B:395:ILE:HB	2.20	0.42
1:C:286:MET:HB2	1:C:286:MET:HE2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:SER:HB3	1:A:356:PRO:HD2	2.01	0.42
1:D:322:PRO:HG3	3:D:1:J25:C15	2.49	0.42
1:B:323:THR:HG22	1:B:399:LEU:HD13	2.00	0.42
1:B:389:HIS:HA	1:B:390:PRO:HA	1.78	0.42
1:B:154:HIS:CD2	1:B:154:HIS:N	2.87	0.42
1:A:130:ASP:HA	7:A:553:HOH:O	2.18	0.42
1:A:98:ASP:OD1	1:A:101:LYS:HD2	2.20	0.42
1:D:204:HIS:HA	1:D:205:PRO:HD3	1.85	0.42
1:B:283:LEU:HG	1:B:383:THR:HG22	2.02	0.42
1:A:326:LEU:HD21	1:A:405:TRP:CE2	2.55	0.42
1:B:370:VAL:HG11	1:B:407:GLN:OE1	2.19	0.42
1:C:373:ILE:HA	1:C:377:VAL:HB	2.01	0.42
1:A:292:VAL:HG12	1:A:293:THR:H	1.84	0.42
1:C:348:ARG:NH2	1:C:360:LYS:HE2	2.32	0.42
1:D:178:THR:OG1	1:D:391:ASP:HB3	2.20	0.42
1:B:359:ASP:O	1:B:363:ALA:HB2	2.18	0.41
1:B:108:ARG:NH1	1:B:108:ARG:CG	2.61	0.41
1:C:204:HIS:HA	1:C:205:PRO:HD3	1.82	0.41
1:C:338:GLU:OE2	1:C:342:ARG:HD2	2.20	0.41
1:C:378:HIS:HB3	1:C:379:PRO:HD3	2.02	0.41
1:C:322:PRO:HA	1:C:329:TYR:CD2	2.55	0.41
1:C:321:ASN:HB2	1:C:322:PRO:HD3	2.03	0.41
1:A:342:ARG:O	1:A:346:ARG:HD2	2.20	0.41
1:B:326:LEU:HD21	1:B:405:TRP:CD2	2.55	0.41
1:A:108:ARG:NH1	1:A:108:ARG:CG	2.82	0.41
1:A:376:ILE:O	1:A:379:PRO:HD2	2.20	0.41
1:C:273:MET:HE3	1:C:276:HIS:HB2	2.02	0.41
1:A:116:ARG:HG3	1:A:147:MET:CE	2.51	0.41
1:B:175:LEU:HA	1:B:175:LEU:HD23	1.81	0.41
1:B:95:GLU:HG3	1:B:108:ARG:HD3	2.01	0.41
1:B:346:ARG:O	1:B:350:ARG:HD2	2.20	0.41
1:B:229:LEU:HA	1:B:229:LEU:HD23	1.86	0.41
1:B:145:TYR:CE1	1:B:241:LEU:HD23	2.56	0.41
1:D:343:GLN:O	1:D:347:GLU:HG3	2.21	0.41
1:C:337:MET:HG3	1:C:365:VAL:CG2	2.48	0.41
1:A:348:ARG:HG3	1:A:349:GLU:N	2.35	0.41
1:C:218:GLU:HG2	1:C:222:MET:CE	2.51	0.41
1:B:326:LEU:O	1:B:330:ARG:HG3	2.21	0.41
1:C:311:GLN:NE2	4:C:7:EDO:H22	2.36	0.41
1:B:262:LYS:HE3	1:B:303:TYR:CE2	2.56	0.41
1:C:252:LEU:HD13	1:C:256:GLN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ALA:HB2	1:B:391:ASP:OD2	2.21	0.41
1:B:307:ILE:HA	1:B:307:ILE:HD12	1.86	0.41
1:C:280:LEU:HD13	1:C:380:LEU:HA	2.03	0.41
1:C:322:PRO:HA	1:C:329:TYR:CG	2.56	0.40
1:D:96:LEU:HD11	1:D:120:VAL:CG1	2.51	0.40
1:D:378:HIS:HA	1:D:399:LEU:HD21	2.03	0.40
1:A:211:PHE:HE2	1:A:347:GLU:HG3	1.85	0.40
1:B:396:LEU:O	1:B:399:LEU:HB3	2.21	0.40
1:A:204:HIS:NE2	1:A:229:LEU:HD13	2.36	0.40
1:C:307:ILE:HG23	1:C:308:GLN:N	2.35	0.40
1:C:222:MET:HG2	1:D:222:MET:HE2	2.02	0.40
1:B:204:HIS:CE1	4:B:3:EDO:H12	2.56	0.40
1:B:207:VAL:HA	1:B:343:GLN:OE1	2.22	0.40
1:D:293:THR:O	1:D:295:SER:O	2.39	0.40
1:C:178:THR:HA	1:C:179:PRO:HD3	1.96	0.40
1:D:131:LEU:HA	1:D:131:LEU:HD23	1.93	0.40
1:B:322:PRO:HG2	1:B:377:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	326/359 (91%)	308 (94%)	14 (4%)	4 (1%)	16	35
1	B	323/359 (90%)	303 (94%)	19 (6%)	1 (0%)	46	72
1	C	323/359 (90%)	306 (95%)	17 (5%)	0	100	100
1	D	322/359 (90%)	310 (96%)	9 (3%)	3 (1%)	21	44
All	All	1294/1436 (90%)	1227 (95%)	59 (5%)	8 (1%)	30	54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	SER
1	B	248	ILE
1	D	349	GLU
1	D	350	ARG
1	A	350	ARG
1	D	351	GLY
1	A	354	ILE
1	A	355	SER

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	299/327 (91%)	290 (97%)	9 (3%)	48	77
1	B	297/327 (91%)	281 (95%)	16 (5%)	27	52
1	C	297/327 (91%)	283 (95%)	14 (5%)	32	60
1	D	296/327 (90%)	286 (97%)	10 (3%)	44	72
All	All	1189/1308 (91%)	1140 (96%)	49 (4%)	37	66

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	LEU
1	A	97	GLU
1	A	147	MET
1	A	178	THR
1	A	222	MET
1	A	286	MET
1	A	299	LEU
1	A	346	ARG
1	A	349	GLU
1	B	92	LEU
1	B	108	ARG
1	B	130	ASP
1	B	139	VAL
1	B	178	THR

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Mol	Chain	Res	Type
1	B	219	LEU
1	B	259	SER
1	B	297	VAL
1	B	298	LEU
1	B	299	LEU
1	B	327	GLN
1	B	346	ARG
1	B	348	ARG
1	B	357	MET
1	B	362	ASN
1	B	396	LEU
1	C	87	GLU
1	C	89	GLU
1	C	90	ASP
1	C	92	LEU
1	C	116	ARG
1	C	147	MET
1	C	178	THR
1	C	219	LEU
1	C	252	LEU
1	C	258	GLN
1	C	286	MET
1	C	289	THR
1	C	297	VAL
1	C	346	ARG
1	D	92	LEU
1	D	99	VAL
1	D	116	ARG
1	D	120	VAL
1	D	178	THR
1	D	219	LEU
1	D	252	LEU
1	D	295	SER
1	D	306	ARG
1	D	342	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	123	HIS
1	A	216	ASN

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Mol	Chain	Res	Type
1	A	245	ASN
1	A	407	GLN
1	B	245	ASN
1	B	258	GLN
1	B	327	GLN
1	B	362	ASN
1	B	389	HIS
1	C	245	ASN
1	C	250	GLN
1	C	258	GLN
1	C	308	GLN
1	D	123	HIS
1	D	127	GLN
1	D	216	ASN
1	D	245	ASN
1	D	278	ASN
1	D	389	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 for Mogul analysis.

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
3	J25	A	1	-	27,30,30	2.20	4 (14%)	19,41,41	4.06	8 (42%)
4	EDO	A	2	-	3,3,3	0.46	0	2,2,2	0.43	0
5	DMS	A	3	-	3,3,3	2.63	1 (33%)	3,3,3	0.55	0
4	EDO	A	4	-	3,3,3	0.46	0	2,2,2	0.56	0
3	J25	B	1	-	27,30,30	2.15	4 (14%)	19,41,41	3.72	6 (31%)
4	EDO	B	2	-	3,3,3	0.45	0	2,2,2	0.52	0
4	EDO	B	3	-	3,3,3	0.55	0	2,2,2	0.19	0
3	J25	C	1	-	27,30,30	2.12	4 (14%)	19,41,41	3.97	8 (42%)
4	EDO	C	2	-	3,3,3	0.38	0	2,2,2	0.64	0
4	EDO	C	3	-	3,3,3	0.54	0	2,2,2	0.18	0
4	EDO	C	4	-	3,3,3	0.47	0	2,2,2	0.48	0
6	EPE	C	5	-	14,15,15	0.36	0	18,20,20	2.35	5 (27%)
4	EDO	C	6	-	3,3,3	0.53	0	2,2,2	0.31	0
4	EDO	C	7	-	3,3,3	0.56	0	2,2,2	0.41	0
3	J25	D	1	-	27,30,30	2.19	5 (18%)	19,41,41	4.17	7 (36%)
4	EDO	D	2	-	3,3,3	0.63	0	2,2,2	0.12	0
4	EDO	D	3	-	3,3,3	0.49	0	2,2,2	0.43	0
4	EDO	D	4	-	3,3,3	0.50	0	2,2,2	0.57	0
4	EDO	D	5	-	3,3,3	0.56	0	2,2,2	0.40	0
4	EDO	D	6	-	3,3,3	0.52	0	2,2,2	0.41	0
4	EDO	D	7	-	3,3,3	0.46	0	2,2,2	0.49	0
4	EDO	D	8	-	3,3,3	0.61	0	2,2,2	0.27	0
4	EDO	D	9	-	3,3,3	0.56	0	2,2,2	0.29	0

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
3	J25	A	1	-	-	2/18/31/31	0/3/3/3
4	EDO	A	2	-	-	0/1/1/1	0/0/0/0
5	DMS	A	3	-	-	0/0/0/0	0/0/0/0
4	EDO	A	4	-	-	0/1/1/1	0/0/0/0
3	J25	B	1	-	-	2/18/31/31	0/3/3/3
4	EDO	B	2	-	-	0/1/1/1	0/0/0/0
4	EDO	B	3	-	-	0/1/1/1	0/0/0/0
3	J25	C	1	-	-	1/18/31/31	0/3/3/3
4	EDO	C	2	-	-	0/1/1/1	0/0/0/0
4	EDO	C	3	-	-	0/1/1/1	0/0/0/0
4	EDO	C	4	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EPE	C	5	-	-	0/9/19/19	0/1/1/1
4	EDO	C	6	-	-	0/1/1/1	0/0/0/0
4	EDO	C	7	-	-	0/1/1/1	0/0/0/0
3	J25	D	1	-	-	2/18/31/31	0/3/3/3
4	EDO	D	2	-	-	0/1/1/1	0/0/0/0
4	EDO	D	3	-	-	0/1/1/1	0/0/0/0
4	EDO	D	4	-	-	0/1/1/1	0/0/0/0
4	EDO	D	5	-	-	0/1/1/1	0/0/0/0
4	EDO	D	6	-	-	0/1/1/1	0/0/0/0
4	EDO	D	7	-	-	0/1/1/1	0/0/0/0
4	EDO	D	8	-	-	0/1/1/1	0/0/0/0
4	EDO	D	9	-	-	0/1/1/1	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	J25	C8-C9	2.11	1.55	1.51
3	D	1	J25	C2-C3	3.22	1.48	1.41
3	C	1	J25	C2-C3	3.64	1.49	1.41
3	B	1	J25	C2-C3	3.83	1.50	1.41
3	A	1	J25	C2-C3	4.08	1.50	1.41
5	A	3	DMS	O-S	4.39	1.80	1.50
3	D	1	J25	O20-C19	4.86	1.45	1.33
3	B	1	J25	C2-C1	4.87	1.49	1.39
3	A	1	J25	O20-C19	4.88	1.45	1.33
3	B	1	J25	O20-C19	5.08	1.45	1.33
3	C	1	J25	O20-C19	5.11	1.45	1.33
3	A	1	J25	C2-C1	5.25	1.50	1.39
3	C	1	J25	C2-C1	5.41	1.50	1.39
3	D	1	J25	C2-C1	5.78	1.51	1.39
3	C	1	J25	O25-C24	6.39	1.46	1.34
3	B	1	J25	O25-C24	6.93	1.47	1.34
3	A	1	J25	O25-C24	7.00	1.47	1.34
3	D	1	J25	O25-C24	7.01	1.47	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	J25	C15-C16-S17	-6.96	105.53	113.23
3	A	1	J25	C15-C16-S17	-6.90	105.59	113.23
3	B	1	J25	C15-C16-S17	-5.99	106.60	113.23
3	C	1	J25	C15-C16-S17	-5.95	106.64	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	J25	O25-C24-O28	-4.91	116.44	124.81
3	C	1	J25	O25-C24-O28	-4.54	117.07	124.81
3	B	1	J25	O25-C24-O28	-4.48	117.17	124.81
3	D	1	J25	C2-C1-C5	-4.12	109.32	113.61
3	A	1	J25	O25-C24-O28	-4.12	117.79	124.81
3	C	1	J25	C2-C1-C5	-3.66	109.80	113.61
3	A	1	J25	C2-C1-C5	-3.36	110.11	113.61
3	B	1	J25	C2-C1-C5	-3.11	110.38	113.61
3	A	1	J25	O28-C24-N7	-2.54	119.50	124.32
6	C	5	EPE	C9-N1-C6	-2.33	105.29	111.27
3	D	1	J25	O20-C19-O23	-2.28	119.48	123.66
3	C	1	J25	O28-C24-N7	-2.18	120.17	124.32
3	A	1	J25	O20-C19-O23	-2.13	119.75	123.66
3	B	1	J25	O20-C19-C2	2.10	117.36	112.45
3	C	1	J25	C21-O20-C19	2.13	121.38	116.46
3	A	1	J25	O20-C19-C2	2.30	117.84	112.45
3	C	1	J25	O20-C19-C2	2.53	118.38	112.45
6	C	5	EPE	C7-N4-C5	2.77	118.36	111.27
6	C	5	EPE	C7-N4-C3	3.24	119.59	111.27
3	C	1	J25	C26-O25-C24	3.79	121.91	115.63
3	D	1	J25	O20-C19-C2	3.83	121.41	112.45
6	C	5	EPE	C5-N4-C3	4.12	117.82	108.90
3	A	1	J25	C26-O25-C24	4.67	123.38	115.63
3	D	1	J25	C26-O25-C24	4.89	123.74	115.63
3	B	1	J25	C26-O25-C24	5.90	125.42	115.63
6	C	5	EPE	O2S-S-C10	6.77	112.68	106.91
3	B	1	J25	O25-C24-N7	11.96	121.22	111.59
3	D	1	J25	O25-C24-N7	13.66	122.60	111.59
3	A	1	J25	O25-C24-N7	13.80	122.71	111.59
3	C	1	J25	O25-C24-N7	13.84	122.74	111.59

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	J25	C26-O25-C24-N7
3	B	1	J25	C26-O25-C24-O28
3	B	1	J25	C26-O25-C24-N7
3	D	1	J25	C26-O25-C24-O28
3	A	1	J25	C26-O25-C24-O28
3	D	1	J25	C26-O25-C24-N7
3	A	1	J25	C26-O25-C24-N7

There are no ring outliers.

11 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	J25	10	0
4	A	4	EDO	1	0
3	B	1	J25	7	0
4	B	3	EDO	3	0
3	C	1	J25	6	0
4	C	2	EDO	1	0
4	C	7	EDO	1	0
3	D	1	J25	4	0
4	D	2	EDO	1	0
4	D	3	EDO	4	0
4	D	6	EDO	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	328/359 (91%)	0.19	23 (7%)	19 17	11, 23, 65, 96	0
1	B	325/359 (90%)	-0.02	9 (2%)	56 55	14, 29, 49, 79	0
1	C	325/359 (90%)	0.14	22 (6%)	20 18	12, 27, 62, 99	0
1	D	324/359 (90%)	-0.10	14 (4%)	39 37	9, 19, 48, 77	0
All	All	1302/1436 (90%)	0.05	68 (5%)	31 28	9, 25, 57, 99	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	ALA	6.7
1	C	357	MET	6.6
1	C	356	PRO	6.2
1	C	362	ASN	6.1
1	A	354	ILE	5.6
1	C	363	ALA	5.5
1	D	362	ASN	5.3
1	D	356	PRO	5.0
1	A	355	SER	5.0
1	A	356	PRO	5.0
1	A	359	ASP	4.8
1	B	356	PRO	4.7
1	D	357	MET	4.6
1	C	355	SER	4.5
1	D	361	HIS	4.5
1	A	362	ASN	4.4
1	A	353	GLU	4.2
1	D	354	ILE	4.2
1	D	363	ALA	3.9
1	D	359	ASP	3.9
1	A	361	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	357	MET	3.8
1	A	375	TYR	3.6
1	D	355	SER	3.6
1	C	359	ASP	3.6
1	C	361	HIS	3.5
1	A	352	MET	3.4
1	B	89	GLU	3.4
1	A	348	ARG	3.3
1	B	361	HIS	3.3
1	C	87	GLU	3.3
1	A	406	TYR	3.1
1	D	367	LYS	3.1
1	A	295	SER	3.1
1	C	408	SER	3.1
1	D	364	SER	3.0
1	B	362	ASN	3.0
1	A	358	CYS	2.9
1	A	289	THR	2.9
1	C	410	ILE	2.9
1	B	88	GLN	2.9
1	D	358	CYS	2.8
1	A	360	LYS	2.8
1	A	367	LYS	2.7
1	A	410	ILE	2.7
1	D	353	GLU	2.7
1	B	90	ASP	2.6
1	C	360	LYS	2.6
1	C	409	THR	2.5
1	C	375	TYR	2.5
1	A	408	SER	2.5
1	C	354	ILE	2.5
1	D	410	ILE	2.5
1	C	353	GLU	2.4
1	C	358	CYS	2.4
1	A	365	VAL	2.4
1	A	364	SER	2.4
1	C	407	GLN	2.3
1	C	364	SER	2.3
1	C	370	VAL	2.3
1	A	409	THR	2.3
1	C	297	VAL	2.2
1	C	86	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	92	LEU	2.2
1	D	348	ARG	2.2
1	B	357	MET	2.2
1	C	295	SER	2.0
1	B	112	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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
4	EDO	B	2	4/4	0.93	0.35	5.80	21,22,32,44	0
3	J25	A	1	28/28	0.85	0.54	4.70	35,53,67,78	0
4	EDO	C	6	4/4	0.92	0.22	4.23	42,46,46,49	0
4	EDO	C	3	4/4	0.90	0.21	4.21	28,31,32,41	0
3	J25	B	1	28/28	0.94	0.32	3.51	26,39,51,55	0
4	EDO	D	2	4/4	0.94	0.21	2.35	18,22,22,27	0
4	EDO	D	7	4/4	0.94	0.18	2.19	23,23,24,35	0
4	EDO	D	6	4/4	0.93	0.18	1.49	15,17,19,21	0
3	J25	C	1	28/28	0.92	0.36	1.42	33,48,55,57	0
6	EPE	C	5	15/15	0.98	0.25	1.13	26,32,52,53	0
4	EDO	C	2	4/4	0.97	0.18	1.04	27,30,30,36	0
4	EDO	B	3	4/4	0.95	0.19	1.02	25,25,30,31	0
4	EDO	D	3	4/4	0.97	0.16	0.99	16,17,25,30	0
3	J25	D	1	28/28	0.94	0.23	0.65	24,38,51,57	0
4	EDO	A	2	4/4	0.98	0.15	0.17	17,18,18,22	0
4	EDO	D	8	4/4	0.98	0.14	-0.31	16,17,20,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	EDO	C	4	4/4	0.93	0.12	-0.87	34,37,38,40	0
2	ZN	A	438	1/1	1.00	0.13	-1.11	18,18,18,18	0
2	ZN	C	438	1/1	1.00	0.10	-2.36	19,19,19,19	0
2	ZN	D	438	1/1	1.00	0.12	-2.47	16,16,16,16	0
2	ZN	C	439	1/1	0.98	0.07	-3.32	37,37,37,37	0
2	ZN	D	439	1/1	0.99	0.10	-3.93	40,40,40,40	0
2	ZN	B	439	1/1	0.99	0.08	-4.08	47,47,47,47	0
2	ZN	A	439	1/1	0.99	0.07	-4.64	39,39,39,39	0
2	ZN	B	438	1/1	1.00	0.09	-5.60	24,24,24,24	0
4	EDO	D	4	4/4	0.97	0.12	-	16,21,21,23	0
4	EDO	D	9	4/4	0.95	0.15	-	27,29,33,35	0
5	DMS	A	3	4/4	0.97	0.14	-	33,35,39,48	0
4	EDO	D	5	4/4	0.86	0.25	-	34,35,37,38	0
4	EDO	C	7	4/4	0.89	0.20	-	34,37,40,45	0
4	EDO	A	4	4/4	0.95	0.19	-	24,25,28,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.