



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:43 AM GMT

PDB ID : 2E4Y
Title : Crystal structure of the extracellular region of the group II metabotropic glutamate receptor complexed with 2R,4R-APDC
Authors : Muto, T.; Tsuchiya, D.; Morikawa, K.; Jingami, H.
Deposited on : 2006-12-17
Resolution : 3.40 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

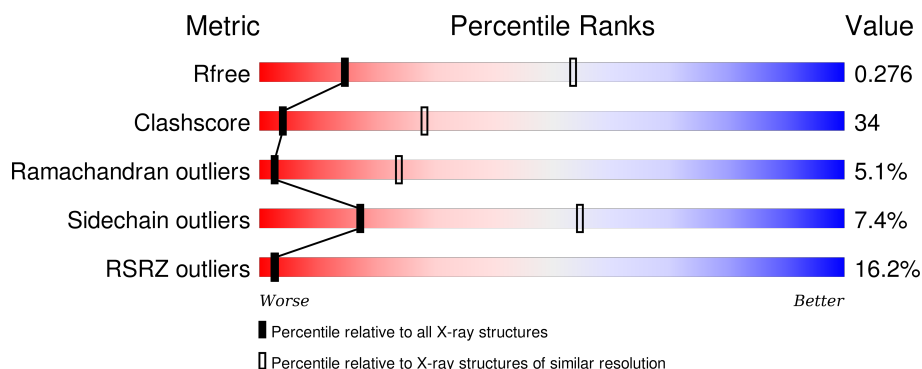
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	555	<div> <div>6%</div> <div>41%</div> <div>45%</div> <div>7%</div> <div>7%</div> </div>
1	B	555	<div> <div>23%</div> <div>39%</div> <div>38%</div> <div>6%</div> <div>17%</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	52A	B	2001	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7823 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 Metabotropic glutamate receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	23	0	0
			4118	2606	709	776	27			
1	B	459	Total	C	N	O	S	23	0	0
			3667	2325	642	685	15			

There are 12 discrepancies between the modelled and reference sequences:

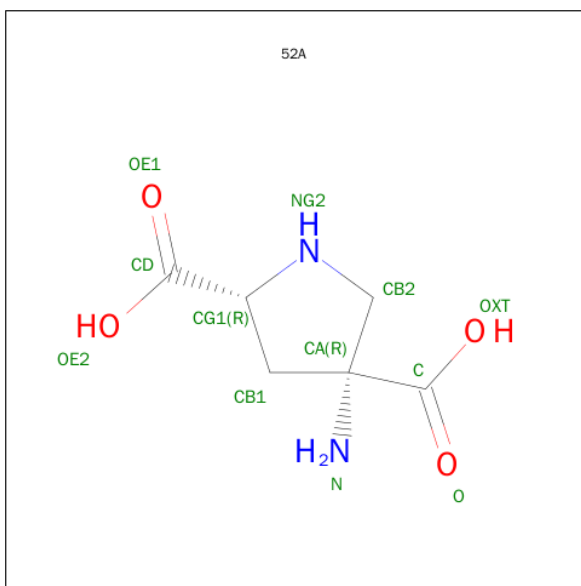
Chain	Residue	Modelled	Actual	Comment	Reference
A	414	GLN	ASN	ENGINEERED	UNP P31422
A	439	GLN	ASN	ENGINEERED	UNP P31422
A	576	LEU	-	CLONING ARTIFACT	UNP P31422
A	577	VAL	-	CLONING ARTIFACT	UNP P31422
A	578	PRO	-	CLONING ARTIFACT	UNP P31422
A	579	ARG	-	CLONING ARTIFACT	UNP P31422
B	414	GLN	ASN	ENGINEERED	UNP P31422
B	439	GLN	ASN	ENGINEERED	UNP P31422
B	576	LEU	-	CLONING ARTIFACT	UNP P31422
B	577	VAL	-	CLONING ARTIFACT	UNP P31422
B	578	PRO	-	CLONING ARTIFACT	UNP P31422
B	579	ARG	-	CLONING ARTIFACT	UNP P31422

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is (2R,4R)-4-AMINOPYRROLIDINE-2,4-DICARBOXYLIC ACID (three-letter code: 52A) (formula: $C_6H_{10}N_2O_4$).

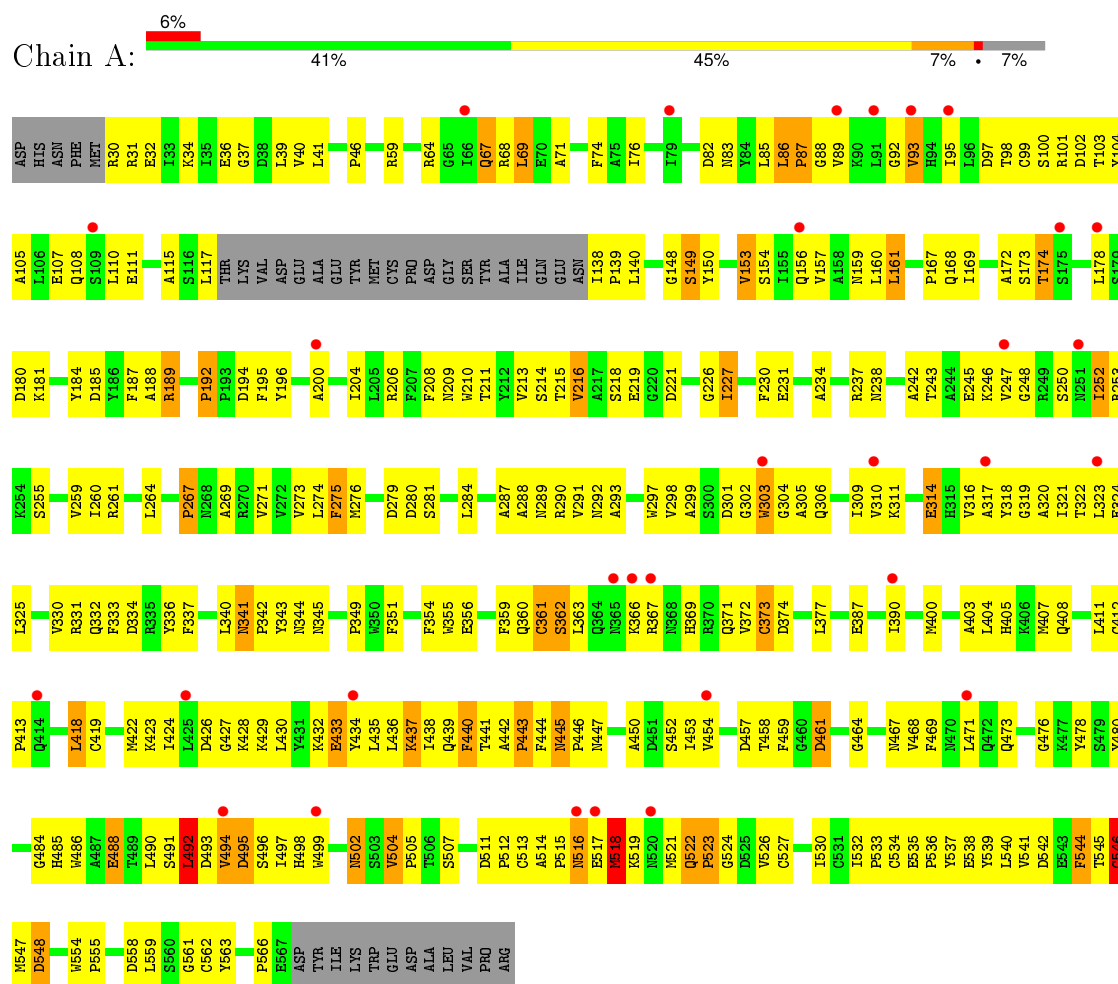


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	6	2	4		
3	B	1	Total	C	N	O	0	0
			12	6	2	4		

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: Metabotropic glutamate receptor 3



GLU	ASP	ALA	ALA	ASP	CYS	D874	Q306	R237	P167	D87
ASP	ALA	ASP	E307	R237	ALA	E307	E307	R237	Q168	T98
LEU	LEU	ASN	S308	I309	ASN	S308	S308	I309	I169	C99
VAL	VAL	GLU	I377	I379	GLU	I377	I379	I379	S170	S100
PRO	PRO	MET	I379	I384	MET	I379	I384	I384	A242	R101
ARG	ARG	LYS	I384	I384	LYS	I384	I384	I384	A172	D102
		ASN	I384	I384	ASN	I384	I384	I384	S173	T103
		ASN	E314	E314	ASN	E314	E314	E314	T114	Y104
		MET	E315	E315	MET	E315	E315	E315	A105	A105
		GLN	E387	E387	GLN	E387	E387	E387	L178	L106
		PRO	S388	S388	PRO	S388	S388	S388	S179	E107
		GLY	K389	K389	GLY	K389	K389	K389	D180	Q108
		ASP	I390	I390	ASP	I390	I390	I390	K181	S109
		VAL	K391	K391	VAL	K391	K391	K391	S250	L110
		CYS	F392	F392	CYS	F392	F392	F392	Y184	E111
		CYS	N395	N395	CYS	N395	N395	N395	D185	F112
		TRP	A396	A396	TRP	A396	A396	A396	Y186	V113
		ILE	V397	V397	ILE	V397	V397	V397	F187	R114
		CYS	V398	V398	CYS	V398	V398	V398	A188	A115
		ILE	A399	A399	ILE	A399	A399	A399	R189	S116
		PRO	M400	M400	PRO	M400	M400	M400	T190	L117
		CYS	A403	A403	CYS	A403	A403	A403	V191	THR
		GLU	L404	L404	GLU	L404	L404	L404	P192	LYS
		TYR	H405	H405	TYR	H405	H405	H405	P193	VAL
		GLU	Q473	Q473	GLU	Q473	Q473	Q473	D194	ASP
		TYR	Q476	Q476	TYR	Q476	Q476	Q476	F195	GLU
		LEU	K477	K477	LEU	K477	K477	K477	Q197	ALA
		VAL	Y478	Y478	VAL	Y478	Y478	Y478	A198	ALA
		ASP	S479	S479	ASP	S479	S479	S479	K199	TYR
		GLU	Y480	Y480	GLU	Y480	Y480	Y480	A200	MET
		PHE	Y483	Y483	PHE	Y483	Y483	Y483	N201	CYS
		THR	G484	G484	THR	G484	G484	G484	A202	PRO
		CYS	H485	H485	CYS	H485	H485	H485	E203	ASP
		NET	W486	W486	NET	W486	W486	W486	I204	GLY
		ASP	A487	A487	ASP	A487	A487	A487	L205	SER
		CYS	E488	E488	CYS	E488	E488	E488	R206	TYR
		GLY	T489	T489	GLY	T489	T489	T489	F207	ALA
		PRO	L490	L490	PRO	L490	L490	L490	F208	ILE
		GLY	S491	S491	GLY	S491	S491	S491	N209	GLN
		GLN	I492	I492	GLN	I492	I492	I492	W210	GLU
		TRP	D493	D493	TRP	D493	D493	D493	T211	ASN
		PRO	W494	W494	PRO	W494	W494	W494	V212	I138
		THR	D495	D495	THR	D495	D495	D495	V213	P139
		ALA	K432	K432	ALA	K432	K432	K432	S214	L140
		ASP	Y434	Y434	ASP	Y434	Y434	Y434	T215	G148
		LEU	L435	L435	LEU	L435	L435	L435	V216	S149
		SER	L436	L436	SER	L436	L436	L436	A217	Y150
		GLY	K437	K437	GLY	K437	K437	K437	S218	V153
		CYS	T438	T438	CYS	T438	T438	T438	G220	S154
		TYR	Q439	Q439	TYR	Q439	Q439	Q439	D221	I155
		ASN	T441	T441	ASN	T441	T441	T441	Y222	Q156
		LEU	W442	W442	LEU	W442	W442	W442	I227	V157
		PRO	S506	S506	PRO	S506	S506	S506	F230	L160
		GLU	Q508	Q508	GLU	Q508	Q508	Q508	E231	L161
		ASP	CYS	CYS	ASP	CYS	CYS	CYS	Q232	R162
		TYR	SER	SER	TYR	SER	SER	SER	E233	L163
		ILE	M445	M445	ILE	M445	M445	M445		
		LYS	P446	P446	LYS	P446	P446	P446		
		TRP			TRP					

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.39Å 91.80Å 112.97Å 90.00° 92.28° 90.00°	Depositor
Resolution (Å)	12.00 – 3.40 84.33 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (12.00-3.40) 99.5 (84.33-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.41Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.284 0.220 , 0.276	Depositor DCC
R_{free} test set	1607 reflections (6.90%)	DCC
Wilson B-factor (Å ²)	122.9	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 137.2	EDS
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 23829 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7823	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: NAG, 52A

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	0.52	0/4212	0.71	2/5704 (0.0%)
1	B	0.37	0/3745	0.65	2/5062 (0.0%)
All	All	0.46	0/7957	0.68	4/10766 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	CYS	CA-CB-SG	-7.22	101.01	114.00
1	A	419	CYS	CA-CB-SG	-7.08	101.25	114.00
1	A	546	CYS	CA-CB-SG	-7.05	101.30	114.00
1	B	412	CYS	CA-CB-SG	-5.14	104.75	114.00

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	4118	0	3994	302	0
1	B	3667	0	3605	227	0
2	A	14	0	13	0	0
3	A	12	0	8	2	0
3	B	12	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7823	0	7628	526	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 34.

All (526) 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:B:437:LYS:HA	1:B:437:LYS:HE3	1.40	1.02
1:B:181:LYS:HE2	1:B:459:PHE:O	1.64	0.98
1:A:437:LYS:HA	1:A:437:LYS:HE3	1.44	0.97
1:A:519:LYS:HD2	1:A:546:CYS:HB2	1.45	0.96
1:A:181:LYS:HE2	1:A:459:PHE:O	1.67	0.95
1:A:514:ALA:HB3	1:A:518:MET:HG3	1.47	0.94
1:B:39:LEU:HD23	1:B:404:LEU:HD13	1.49	0.94
1:A:493:ASP:OD2	1:A:496:SER:HB3	1.69	0.93
1:A:39:LEU:HD23	1:A:404:LEU:HD13	1.51	0.93
1:B:356:GLU:HA	1:B:361:CYS:HB2	1.50	0.92
1:A:538:GLU:HB3	1:A:548:ASP:HA	1.51	0.92
1:A:341:ASN:HD22	1:A:343:TYR:H	1.16	0.90
1:A:442:ALA:O	1:A:444:PHE:N	2.08	0.87
1:A:213:VAL:HG12	1:A:271:VAL:HB	1.57	0.86
1:B:299:ALA:HB3	1:B:322:THR:HG22	1.56	0.86
1:B:276:MET:HE3	1:B:281:SER:HA	1.56	0.86
1:B:341:ASN:HD22	1:B:343:TYR:H	1.17	0.85
1:B:216:VAL:HG13	1:B:274:LEU:HD23	1.59	0.85
1:A:356:GLU:HA	1:A:361:CYS:HB2	1.59	0.84
1:B:252:ILE:HG22	1:B:253:ARG:H	1.42	0.84
1:B:213:VAL:HG12	1:B:271:VAL:HB	1.61	0.82
1:B:493:ASP:OD2	1:B:496:SER:HB3	1.80	0.82
1:A:252:ILE:HG22	1:A:253:ARG:H	1.43	0.81
1:A:366:LYS:HG2	1:A:367:ARG:H	1.45	0.80
1:B:442:ALA:O	1:B:444:PHE:N	2.16	0.79
1:A:216:VAL:HG13	1:A:274:LEU:HD23	1.65	0.79
1:B:366:LYS:HG2	1:B:367:ARG:H	1.46	0.77
1:A:310:VAL:HG13	1:A:317:ALA:HB3	1.66	0.77
1:A:148:GLY:HA3	1:A:154:SER:OG	1.85	0.77
1:A:494:VAL:C	1:A:496:SER:H	1.87	0.77
1:B:287:ALA:HA	1:B:290:ARG:NH1	1.99	0.76
1:A:515:PRO:HG2	1:A:516:ASN:H	1.49	0.76
1:B:216:VAL:HA	1:B:245:GLU:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:THR:HG23	1:B:452:SER:O	1.86	0.75
1:B:362:SER:O	1:B:363:LEU:HD22	1.87	0.74
1:A:310:VAL:HG12	1:A:314:GLU:HA	1.70	0.74
1:B:310:VAL:HG12	1:B:314:GLU:HA	1.70	0.74
1:A:540:LEU:N	1:A:540:LEU:HD12	2.02	0.73
1:A:442:ALA:C	1:A:444:PHE:H	1.90	0.73
1:A:287:ALA:HA	1:A:290:ARG:NH1	2.04	0.73
1:A:276:MET:HE3	1:A:281:SER:HA	1.70	0.72
1:B:148:GLY:HA3	1:B:154:SER:OG	1.90	0.72
1:A:216:VAL:HA	1:A:245:GLU:O	1.90	0.72
1:B:311:LYS:HA	1:B:314:GLU:OE2	1.89	0.71
1:A:490:LEU:HG	1:A:492:LEU:HD22	1.72	0.71
1:A:299:ALA:HB3	1:A:322:THR:HG22	1.72	0.71
1:A:372:VAL:HG22	1:A:373:CYS:H	1.56	0.71
1:A:538:GLU:CB	1:A:548:ASP:HA	2.21	0.70
1:A:74:PHE:HB2	1:A:336:TYR:CE2	2.26	0.70
1:A:362:SER:O	1:A:363:LEU:HD22	1.91	0.70
1:B:74:PHE:HB2	1:B:336:TYR:CE2	2.27	0.70
1:A:535:GLU:HA	1:A:535:GLU:OE2	1.91	0.69
1:A:187:PHE:HE2	1:A:189:ARG:HD2	1.57	0.69
1:A:408:GLN:HA	1:A:422:MET:HE2	1.74	0.68
1:A:438:ILE:HG23	1:A:453:ILE:HD12	1.75	0.68
1:A:521:MET:HB2	1:A:530:ILE:HG13	1.75	0.68
1:A:441:THR:HG23	1:A:452:SER:O	1.92	0.68
1:B:310:VAL:HG13	1:B:317:ALA:HB3	1.74	0.68
1:B:255:SER:O	1:B:259:VAL:HG23	1.93	0.68
1:A:213:VAL:CG1	1:A:271:VAL:HB	2.24	0.67
1:B:408:GLN:HA	1:B:422:MET:HE2	1.75	0.67
1:A:311:LYS:HA	1:A:314:GLU:OE2	1.94	0.67
1:A:342:PRO:HD3	1:A:355:TRP:CD2	2.31	0.66
1:A:518:MET:HA	1:A:532:ILE:O	1.96	0.66
1:B:115:ALA:HB1	1:B:140:LEU:O	1.96	0.66
1:A:342:PRO:HD3	1:A:355:TRP:CE3	2.31	0.66
1:B:342:PRO:HD3	1:B:355:TRP:CD2	2.31	0.66
1:B:442:ALA:C	1:B:444:PHE:H	1.96	0.65
1:A:115:ALA:HB1	1:A:140:LEU:O	1.95	0.65
1:A:255:SER:O	1:A:259:VAL:HG23	1.96	0.65
1:B:252:ILE:N	1:B:252:ILE:HD12	2.12	0.65
1:A:216:VAL:HG13	1:A:274:LEU:CD2	2.26	0.65
1:A:87:PRO:HG2	1:A:88:GLY:H	1.61	0.65
1:B:98:THR:HB	1:B:105:ALA:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ASN:ND2	1:A:343:TYR:H	1.93	0.65
1:A:298:VAL:HA	1:A:321:ILE:O	1.98	0.64
1:B:372:VAL:HG22	1:B:373:CYS:H	1.63	0.64
1:A:274:LEU:HD11	1:A:297:TRP:CE3	2.32	0.64
1:A:518:MET:HA	1:A:533:PRO:HA	1.80	0.63
1:B:366:LYS:HE2	1:B:369:HIS:HD2	1.64	0.63
1:B:297:TRP:HB2	1:B:320:ALA:HB1	1.81	0.63
1:A:264:LEU:O	1:A:267:PRO:HD3	1.99	0.63
1:B:494:VAL:C	1:B:496:SER:H	1.98	0.63
1:A:64:ARG:HD3	3:A:1001:52A:OE1	1.99	0.62
1:B:264:LEU:O	1:B:267:PRO:HD3	1.98	0.62
1:B:260:ILE:CD1	1:B:288:ALA:HB2	2.29	0.62
1:B:41:LEU:HD22	1:B:400:MET:HG2	1.82	0.62
1:A:490:LEU:HD12	1:A:491:SER:H	1.65	0.62
1:A:366:LYS:HE2	1:A:369:HIS:HD2	1.63	0.62
1:B:86:LEU:CD1	1:B:405:HIS:HA	2.30	0.61
1:B:323:LEU:HD23	1:B:468:VAL:HA	1.82	0.61
1:B:169:ILE:HA	1:B:188:ALA:O	2.00	0.61
1:A:252:ILE:N	1:A:252:ILE:HD12	2.16	0.61
1:B:216:VAL:HB	1:B:245:GLU:HB2	1.83	0.61
1:A:64:ARG:O	1:A:68:ARG:HD2	2.00	0.61
1:B:32:GLU:OE2	1:B:34:LYS:HE3	2.01	0.60
1:B:473:GLN:NE2	1:B:476:GLY:H	1.99	0.60
1:B:64:ARG:HD3	3:B:2001:52A:OE1	2.01	0.60
1:A:260:ILE:CD1	1:A:288:ALA:HB2	2.30	0.60
1:A:340:LEU:HD22	1:A:345:ASN:ND2	2.16	0.60
1:A:467:ASN:HB3	1:A:469:PHE:HE1	1.66	0.60
1:A:246:LYS:O	1:A:246:LYS:HG3	2.00	0.60
1:B:490:LEU:HD12	1:B:491:SER:H	1.66	0.60
1:B:340:LEU:HD22	1:B:345:ASN:ND2	2.17	0.60
1:A:227:ILE:HD13	1:A:230:PHE:HB3	1.84	0.60
1:B:87:PRO:HG2	1:B:88:GLY:H	1.65	0.60
1:A:490:LEU:CD1	1:A:491:SER:H	2.15	0.60
1:B:298:VAL:HA	1:B:321:ILE:O	2.01	0.60
1:B:342:PRO:HD3	1:B:355:TRP:CE3	2.37	0.59
1:A:178:LEU:HA	1:A:184:TYR:CD1	2.38	0.59
1:A:110:LEU:HD21	1:B:113:VAL:HG23	1.83	0.59
1:B:341:ASN:ND2	1:B:343:TYR:H	1.96	0.59
1:A:424:ILE:HG13	1:A:424:ILE:O	2.01	0.59
1:A:169:ILE:HA	1:A:188:ALA:O	2.02	0.58
1:B:82:ASP:OD2	1:B:83:ASN:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:VAL:O	1:B:298:VAL:HG12	2.04	0.58
1:A:138:ILE:N	1:A:139:PRO:HD2	2.18	0.58
1:A:535:GLU:O	1:A:537:TYR:N	2.36	0.58
1:A:341:ASN:HA	1:A:355:TRP:CZ3	2.38	0.58
1:B:64:ARG:O	1:B:68:ARG:HD2	2.02	0.58
1:A:493:ASP:O	1:A:495:ASP:N	2.36	0.58
1:A:323:LEU:HD23	1:A:468:VAL:HA	1.85	0.58
1:B:178:LEU:HA	1:B:184:TYR:CD1	2.38	0.58
1:A:341:ASN:HD22	1:A:343:TYR:N	1.94	0.58
1:A:490:LEU:CG	1:A:491:SER:H	2.17	0.58
1:B:430:LEU:O	1:B:434:TYR:HB2	2.04	0.58
1:A:517:GLU:HG2	1:A:533:PRO:HB2	1.86	0.58
1:A:39:LEU:HD22	1:A:89:VAL:HG11	1.85	0.58
1:A:41:LEU:HD22	1:A:400:MET:HG2	1.85	0.58
1:B:438:ILE:HG23	1:B:453:ILE:HD12	1.85	0.57
1:B:216:VAL:HG13	1:B:274:LEU:CD2	2.33	0.57
1:B:411:LEU:HD12	1:B:422:MET:HG2	1.86	0.57
1:B:362:SER:HA	1:B:366:LYS:HD2	1.87	0.57
1:A:86:LEU:CD1	1:A:405:HIS:HA	2.35	0.57
1:B:493:ASP:O	1:B:495:ASP:N	2.37	0.57
1:A:108:GLN:O	1:A:111:GLU:HB2	2.05	0.57
1:A:98:THR:HB	1:A:105:ALA:HB2	1.86	0.57
1:A:539:TYR:CD1	1:A:540:LEU:N	2.73	0.57
1:B:227:ILE:HD13	1:B:230:PHE:HB3	1.87	0.57
1:A:555:PRO:HA	1:A:561:GLY:O	2.05	0.57
1:B:252:ILE:HD12	1:B:252:ILE:H	1.70	0.56
1:B:213:VAL:CG1	1:B:271:VAL:HB	2.32	0.56
1:B:138:ILE:N	1:B:139:PRO:HD2	2.20	0.56
1:A:519:LYS:HE2	1:A:521:MET:SD	2.45	0.56
1:A:490:LEU:HG	1:A:491:SER:N	2.20	0.56
1:B:341:ASN:HD22	1:B:343:TYR:N	1.96	0.56
1:A:539:TYR:C	1:A:540:LEU:HD12	2.25	0.56
1:A:298:VAL:HG12	1:A:298:VAL:O	2.06	0.56
1:A:473:GLN:NE2	1:A:476:GLY:H	2.03	0.56
1:B:424:ILE:HG13	1:B:424:ILE:O	2.06	0.56
1:A:453:ILE:HG13	1:A:453:ILE:O	2.05	0.55
1:A:274:LEU:HD22	1:A:276:MET:HE1	1.88	0.55
1:B:279:ASP:OD1	1:B:280:ASP:N	2.39	0.55
1:B:437:LYS:HE2	1:B:438:ILE:H	1.71	0.55
1:A:216:VAL:HB	1:A:245:GLU:HB2	1.87	0.55
1:B:260:ILE:HD12	1:B:288:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:SER:N	1:B:276:MET:HG2	2.22	0.54
1:A:40:VAL:HG13	1:A:92:GLY:C	2.28	0.54
1:A:540:LEU:HG	1:A:546:CYS:SG	2.47	0.54
1:A:271:VAL:HG23	1:A:507:SER:HB2	1.89	0.54
1:A:430:LEU:O	1:A:434:TYR:HB2	2.07	0.54
1:A:260:ILE:HD12	1:A:288:ALA:HB2	1.88	0.54
1:B:31:ARG:HD2	1:B:349:PRO:HB2	1.88	0.54
1:B:437:LYS:HA	1:B:437:LYS:CE	2.25	0.54
1:B:400:MET:CE	1:B:400:MET:HA	2.37	0.54
1:B:437:LYS:CA	1:B:437:LYS:HE3	2.27	0.54
1:A:153:VAL:O	1:A:157:VAL:HG23	2.07	0.54
1:A:156:GLN:HA	1:A:156:GLN:OE1	2.06	0.54
1:A:192:PRO:HG3	1:A:464:GLY:HA2	1.90	0.54
1:B:214:SER:OG	1:B:243:THR:HG22	2.07	0.54
1:A:211:THR:HG22	1:A:527:CYS:SG	2.48	0.54
1:B:366:LYS:HE2	1:B:369:HIS:CD2	2.43	0.53
1:A:274:LEU:HD22	1:A:276:MET:CE	2.38	0.53
1:A:494:VAL:C	1:A:496:SER:N	2.58	0.53
1:A:297:TRP:HB2	1:A:320:ALA:HB1	1.90	0.53
1:A:168:GLN:C	1:A:169:ILE:HG13	2.29	0.53
1:A:200:ALA:O	1:A:204:ILE:HG13	2.09	0.53
1:A:226:GLY:HA3	1:A:275:PHE:CE2	2.44	0.53
1:A:169:ILE:HD11	1:A:400:MET:SD	2.48	0.53
1:B:102:ASP:OD2	1:B:103:THR:N	2.37	0.53
1:B:461:ASP:N	1:B:461:ASP:OD2	2.38	0.53
1:B:74:PHE:HB2	1:B:336:TYR:CD2	2.43	0.53
1:A:519:LYS:HE3	1:A:544:PHE:O	2.08	0.53
1:A:362:SER:HA	1:A:366:LYS:HD2	1.90	0.53
1:A:491:SER:C	1:A:492:LEU:HD22	2.29	0.53
1:B:453:ILE:HG13	1:B:453:ILE:O	2.08	0.53
1:A:82:ASP:OD2	1:A:83:ASN:N	2.41	0.53
1:A:490:LEU:CG	1:A:491:SER:N	2.73	0.52
1:B:214:SER:OG	1:B:242:ALA:HB3	2.10	0.52
1:A:442:ALA:C	1:A:444:PHE:N	2.59	0.52
1:B:76:ILE:HG13	1:B:93:VAL:HG11	1.91	0.52
1:A:160:LEU:HB2	1:B:163:LEU:HD23	1.92	0.52
1:A:515:PRO:CG	1:A:516:ASN:H	2.21	0.52
1:B:185:ASP:OD2	1:B:185:ASP:N	2.42	0.52
1:A:366:LYS:HE2	1:A:369:HIS:CD2	2.42	0.52
1:A:86:LEU:HD13	1:A:405:HIS:HA	1.91	0.52
1:A:490:LEU:HG	1:A:491:SER:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ASN:HB2	1:A:342:PRO:HD2	1.91	0.52
1:A:252:ILE:HD12	1:A:252:ILE:H	1.73	0.52
1:A:74:PHE:HB2	1:A:336:TYR:CD2	2.45	0.52
1:B:260:ILE:HD11	1:B:288:ALA:HB2	1.92	0.52
1:B:191:VAL:HG12	1:B:392:PHE:CD2	2.45	0.52
1:A:31:ARG:HD2	1:A:349:PRO:HB2	1.92	0.52
1:A:542:ASP:OD2	1:A:545:THR:N	2.40	0.52
1:B:252:ILE:HG22	1:B:253:ARG:N	2.21	0.52
1:A:32:GLU:OE2	1:A:34:LYS:HE3	2.10	0.52
1:B:314:GLU:CD	1:B:314:GLU:H	2.13	0.51
1:B:297:TRP:HB2	1:B:320:ALA:CB	2.39	0.51
1:A:46:PRO:HD3	1:A:149:SER:HB2	1.92	0.51
1:B:418:LEU:HD22	1:B:422:MET:HE3	1.93	0.51
1:A:554:TRP:CG	1:A:555:PRO:HD2	2.45	0.51
1:B:117:LEU:HD12	1:B:117:LEU:N	2.24	0.51
1:A:435:LEU:C	1:A:437:LYS:H	2.13	0.51
1:A:76:ILE:HG13	1:A:93:VAL:HG11	1.91	0.51
1:B:169:ILE:HD11	1:B:400:MET:SD	2.50	0.51
1:A:411:LEU:HD12	1:A:422:MET:HG2	1.93	0.51
1:A:428:LYS:O	1:A:432:LYS:HG2	2.10	0.51
1:A:86:LEU:HG	1:A:89:VAL:HB	1.93	0.51
1:A:521:MET:HB2	1:A:530:ILE:CG1	2.41	0.51
1:B:411:LEU:C	1:B:412:CYS:SG	2.89	0.51
1:B:301:ASP:HA	1:B:323:LEU:O	2.11	0.51
1:B:204:ILE:HG22	1:B:205:LEU:HD23	1.92	0.51
1:B:291:VAL:O	1:B:293:ALA:N	2.44	0.51
1:B:435:LEU:C	1:B:437:LYS:H	2.14	0.51
1:A:372:VAL:HG22	1:A:373:CYS:N	2.23	0.51
1:B:490:LEU:HG	1:B:492:LEU:HD22	1.92	0.51
1:B:205:LEU:HD22	1:B:210:TRP:CE3	2.46	0.51
1:B:108:GLN:O	1:B:111:GLU:HB2	2.10	0.51
1:A:305:ALA:HA	1:A:480:TYR:CE2	2.47	0.50
1:B:442:ALA:C	1:B:444:PHE:N	2.64	0.50
1:A:332:GLN:OE1	1:A:332:GLN:N	2.40	0.50
1:A:494:VAL:O	1:A:496:SER:N	2.44	0.50
1:B:246:LYS:HG3	1:B:246:LYS:O	2.12	0.50
1:B:486:TRP:CH2	1:B:488:GLU:HA	2.47	0.50
1:A:558:ASP:O	1:A:559:LEU:HB2	2.11	0.50
1:A:341:ASN:C	1:A:341:ASN:HD22	2.14	0.50
1:B:274:LEU:HD22	1:B:276:MET:CE	2.42	0.50
1:A:411:LEU:C	1:A:412:CYS:SG	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ILE:O	1:B:94:HIS:HA	2.12	0.50
1:A:461:ASP:N	1:A:461:ASP:OD2	2.39	0.50
1:A:157:VAL:HG12	1:A:161:LEU:HD22	1.93	0.50
1:A:185:ASP:N	1:A:185:ASP:OD2	2.44	0.50
1:A:59:ARG:HB2	1:A:59:ARG:HH11	1.76	0.50
1:A:359:PHE:O	1:A:360:GLN:HB2	2.12	0.50
1:B:314:GLU:HG3	1:B:478:TYR:CD2	2.47	0.50
1:B:76:ILE:HG13	1:B:93:VAL:CG1	2.42	0.50
1:B:195:PHE:HD2	1:B:196:TYR:CE1	2.30	0.50
1:B:362:SER:C	1:B:363:LEU:HD22	2.32	0.49
1:A:322:THR:O	1:A:469:PHE:HB2	2.12	0.49
1:A:261:ARG:O	1:A:264:LEU:HB2	2.11	0.49
1:B:341:ASN:HA	1:B:355:TRP:CZ3	2.46	0.49
1:B:156:GLN:OE1	1:B:156:GLN:HA	2.12	0.49
1:A:41:LEU:CD2	1:A:400:MET:HG2	2.42	0.49
1:A:301:ASP:HA	1:A:323:LEU:O	2.12	0.49
1:A:515:PRO:O	1:A:517:GLU:N	2.46	0.49
1:A:457:ASP:HB2	1:A:461:ASP:OD2	2.13	0.49
1:A:64:ARG:HG2	1:A:68:ARG:CZ	2.42	0.49
1:A:301:ASP:O	1:A:304:GLY:N	2.46	0.49
1:A:522:GLN:HE21	1:A:522:GLN:HA	1.77	0.49
1:B:437:LYS:CE	1:B:438:ILE:H	2.25	0.49
1:A:437:LYS:CA	1:A:437:LYS:HE3	2.30	0.49
1:A:260:ILE:HD11	1:A:288:ALA:HB2	1.94	0.49
1:A:117:LEU:N	1:A:117:LEU:HD12	2.26	0.49
1:A:434:TYR:O	1:A:437:LYS:HB2	2.13	0.49
1:B:205:LEU:HD22	1:B:210:TRP:HE3	1.78	0.49
1:B:387:GLU:HB3	1:B:390:ILE:HG12	1.95	0.49
1:A:544:PHE:N	1:A:544:PHE:CD1	2.81	0.48
1:A:341:ASN:ND2	1:A:341:ASN:C	2.66	0.48
1:A:314:GLU:CD	1:A:314:GLU:H	2.15	0.48
1:B:192:PRO:HG3	1:B:464:GLY:HA2	1.95	0.48
1:B:372:VAL:HG22	1:B:373:CYS:N	2.27	0.48
1:A:306:GLN:HB2	1:A:309:ILE:HD12	1.94	0.48
1:A:159:ASN:HB3	1:B:163:LEU:HD11	1.95	0.48
1:A:289:ASN:CB	1:A:316:VAL:HG21	2.44	0.48
1:B:219:GLU:HB2	1:B:248:GLY:HA2	1.94	0.48
1:B:187:PHE:HE2	1:B:189:ARG:HD2	1.78	0.48
1:A:355:TRP:CE2	1:A:359:PHE:CE1	3.01	0.48
1:B:46:PRO:HD3	1:B:149:SER:HB2	1.95	0.48
1:B:30:ARG:HG2	1:B:30:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:VAL:HG13	1:B:444:PHE:HB3	1.94	0.48
1:A:445:ASN:ND2	1:A:447:ASN:O	2.47	0.48
1:A:40:VAL:HG12	1:A:41:LEU:N	2.29	0.48
1:A:433:GLU:O	1:A:433:GLU:HG3	2.14	0.48
1:A:563:TYR:CD1	1:A:563:TYR:O	2.66	0.48
1:A:279:ASP:OD1	1:A:280:ASP:N	2.46	0.48
1:A:554:TRP:O	1:A:562:CYS:HA	2.14	0.48
1:A:426:ASP:O	1:A:427:GLY:C	2.52	0.48
1:A:36:GLU:HG2	1:A:37:GLY:N	2.28	0.48
1:A:173:SER:HA	3:A:1001:52A:OXT	2.13	0.48
1:B:36:GLU:HG2	1:B:37:GLY:N	2.28	0.48
1:A:493:ASP:CG	1:A:496:SER:HB3	2.33	0.48
1:B:64:ARG:CZ	1:B:306:GLN:NE2	2.77	0.48
1:B:440:PHE:CD2	1:B:453:ILE:HG22	2.49	0.48
1:B:289:ASN:HA	1:B:316:VAL:HG21	1.96	0.48
1:A:486:TRP:CH2	1:A:488:GLU:HA	2.49	0.48
1:B:322:THR:O	1:B:469:PHE:HB2	2.14	0.48
1:B:200:ALA:HA	1:B:486:TRP:CD1	2.49	0.48
1:B:331:ARG:O	1:B:334:ASP:HB2	2.13	0.48
1:A:284:LEU:HD13	1:A:284:LEU:C	2.34	0.47
1:A:306:GLN:HB2	1:A:309:ILE:CD1	2.45	0.47
1:A:59:ARG:NH1	1:A:59:ARG:CB	2.76	0.47
1:A:535:GLU:C	1:A:537:TYR:H	2.18	0.47
1:A:276:MET:HB2	1:A:281:SER:OG	2.14	0.47
1:B:284:LEU:C	1:B:284:LEU:HD13	2.34	0.47
1:A:492:LEU:HD23	1:A:492:LEU:N	2.30	0.47
1:A:138:ILE:N	1:A:139:PRO:CD	2.78	0.47
1:A:101:ARG:HD3	1:A:103:THR:OG1	2.14	0.47
1:A:99:CYS:HB2	1:A:104:TYR:CD2	2.50	0.47
1:A:99:CYS:SG	1:A:104:TYR:CE2	3.07	0.47
1:A:324:GLU:HG3	1:A:325:LEU:N	2.29	0.47
1:B:324:GLU:HG3	1:B:325:LEU:N	2.29	0.47
1:B:445:ASN:ND2	1:B:447:ASN:O	2.47	0.47
1:A:403:ALA:HB2	1:A:434:TYR:CD1	2.50	0.47
1:A:514:ALA:CB	1:A:518:MET:HG3	2.32	0.47
1:A:484:GLY:HA3	1:A:492:LEU:HA	1.97	0.47
1:A:187:PHE:CE2	1:A:189:ARG:HB3	2.49	0.47
1:B:337:PHE:CD1	1:B:340:LEU:HD12	2.48	0.47
1:B:227:ILE:O	1:B:231:GLU:HG3	2.15	0.47
1:B:59:ARG:HH11	1:B:59:ARG:HB2	1.79	0.47
1:A:71:ALA:HA	1:A:333:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:TYR:HE1	1:A:541:VAL:HA	1.80	0.47
1:B:359:PHE:HB3	1:B:377:LEU:HD21	1.97	0.47
1:A:219:GLU:HB2	1:A:248:GLY:HA2	1.97	0.47
1:A:330:VAL:HG13	1:A:444:PHE:HB3	1.97	0.47
1:A:68:ARG:NH1	1:A:149:SER:OG	2.48	0.47
1:A:303:TRP:C	1:A:303:TRP:CD1	2.87	0.47
1:B:456:PHE:HB3	1:B:460:GLY:HA2	1.97	0.47
1:A:76:ILE:HG13	1:A:93:VAL:CG1	2.44	0.47
1:A:499:TRP:CD2	1:A:505:PRO:HD3	2.50	0.47
1:B:494:VAL:C	1:B:496:SER:N	2.68	0.47
1:B:490:LEU:CD1	1:B:491:SER:H	2.27	0.47
1:A:40:VAL:HG13	1:A:92:GLY:O	2.15	0.47
1:A:102:ASP:OD2	1:A:103:THR:N	2.41	0.47
1:A:540:LEU:HB3	1:A:542:ASP:O	2.15	0.46
1:A:227:ILE:O	1:A:231:GLU:HG3	2.16	0.46
1:B:69:LEU:HD23	1:B:69:LEU:C	2.35	0.46
1:A:441:THR:O	1:A:442:ALA:C	2.54	0.46
1:B:467:ASN:HB3	1:B:469:PHE:HE1	1.79	0.46
1:A:497:ILE:HG21	1:A:499:TRP:CZ2	2.50	0.46
1:A:519:LYS:HG2	1:A:532:ILE:O	2.16	0.46
1:B:441:THR:O	1:B:442:ALA:C	2.54	0.46
1:A:535:GLU:C	1:A:537:TYR:N	2.69	0.46
1:B:274:LEU:HD22	1:B:276:MET:HE1	1.97	0.46
1:B:341:ASN:HD22	1:B:341:ASN:C	2.19	0.46
1:A:540:LEU:CD1	1:A:540:LEU:N	2.76	0.46
1:B:157:VAL:HG12	1:B:161:LEU:HD22	1.96	0.46
1:B:341:ASN:HB2	1:B:342:PRO:HD2	1.98	0.46
1:A:310:VAL:HG21	1:A:471:LEU:HD22	1.97	0.46
1:A:86:LEU:HD13	1:A:405:HIS:CA	2.46	0.46
1:A:211:THR:HG23	1:A:238:ASN:O	2.16	0.46
1:A:491:SER:C	1:A:492:LEU:CD2	2.84	0.46
1:B:195:PHE:HD2	1:B:196:TYR:HE1	1.64	0.46
1:B:107:GLU:O	1:B:110:LEU:HB2	2.16	0.46
1:A:492:LEU:N	1:A:492:LEU:CD2	2.79	0.46
1:A:174:THR:HB	1:A:194:ASP:OD1	2.15	0.46
1:A:206:ARG:HD2	1:A:237:ARG:HB3	1.97	0.46
1:B:287:ALA:HA	1:B:290:ARG:CZ	2.44	0.46
1:A:400:MET:HA	1:A:400:MET:CE	2.45	0.46
1:B:196:TYR:N	1:B:196:TYR:CD1	2.84	0.46
1:B:69:LEU:CD2	1:B:69:LEU:C	2.85	0.46
1:A:230:PHE:CZ	1:A:273:VAL:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:GLU:O	1:B:433:GLU:HG3	2.15	0.45
1:B:491:SER:O	1:B:492:LEU:HB3	2.16	0.45
1:A:539:TYR:HD1	1:A:540:LEU:N	2.15	0.45
1:A:231:GLU:O	1:A:234:ALA:HB3	2.15	0.45
1:A:412:CYS:HA	1:A:413:PRO:HD2	1.73	0.45
1:B:196:TYR:HD1	1:B:196:TYR:N	2.14	0.45
1:B:403:ALA:HB2	1:B:434:TYR:CD1	2.51	0.45
1:B:167:PRO:HG3	1:B:430:LEU:HD23	1.98	0.45
1:B:374:ASP:O	1:B:377:LEU:HB2	2.17	0.45
1:B:86:LEU:HD13	1:B:405:HIS:CA	2.46	0.45
1:A:435:LEU:O	1:A:437:LYS:N	2.49	0.45
1:A:361:CYS:HB3	1:A:362:SER:H	1.39	0.45
1:B:86:LEU:HD13	1:B:405:HIS:HA	1.99	0.45
1:B:110:LEU:HA	1:B:110:LEU:HD12	1.77	0.45
1:A:437:LYS:CE	1:A:438:ILE:H	2.30	0.45
1:A:437:LYS:HE2	1:A:438:ILE:H	1.80	0.45
1:B:303:TRP:C	1:B:303:TRP:CD1	2.91	0.45
1:B:86:LEU:HG	1:B:89:VAL:HB	1.98	0.45
1:A:535:GLU:O	1:A:538:GLU:HG2	2.17	0.45
1:A:64:ARG:CZ	1:A:306:GLN:NE2	2.80	0.45
1:A:314:GLU:HG3	1:A:478:TYR:CD2	2.53	0.44
1:B:426:ASP:HB3	1:B:429:LYS:HB2	1.99	0.44
1:B:341:ASN:C	1:B:341:ASN:ND2	2.71	0.44
1:B:138:ILE:N	1:B:139:PRO:CD	2.79	0.44
1:A:387:GLU:HB3	1:A:390:ILE:HG12	1.99	0.44
1:A:517:GLU:HB3	1:A:518:MET:H	1.61	0.44
1:A:87:PRO:HG2	1:A:88:GLY:N	2.30	0.44
1:A:30:ARG:HH11	1:A:30:ARG:HG2	1.81	0.44
1:A:442:ALA:HA	1:A:443:PRO:HD2	1.63	0.44
1:A:59:ARG:CB	1:A:59:ARG:HH11	2.30	0.44
1:B:178:LEU:O	1:B:181:LYS:NZ	2.48	0.44
1:A:355:TRP:CE2	1:A:359:PHE:HE1	2.36	0.44
1:B:97:ASP:OD1	1:B:98:THR:N	2.50	0.44
1:A:323:LEU:HD21	1:A:468:VAL:HG22	1.99	0.44
1:A:359:PHE:HB3	1:A:377:LEU:HD21	1.99	0.44
1:B:218:SER:OG	1:B:280:ASP:HB2	2.18	0.44
1:B:422:MET:O	1:B:423:LYS:C	2.55	0.44
1:B:48:ASN:OD1	1:B:60:ILE:HD13	2.17	0.44
1:B:442:ALA:HA	1:B:443:PRO:HD2	1.71	0.44
1:A:490:LEU:HG	1:A:492:LEU:CD2	2.45	0.44
1:B:86:LEU:HD13	1:B:405:HIS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ASP:HB2	1:B:461:ASP:OD2	2.17	0.44
1:A:374:ASP:O	1:A:377:LEU:HB2	2.18	0.44
1:A:287:ALA:HA	1:A:290:ARG:CZ	2.47	0.44
1:A:473:GLN:NE2	1:A:476:GLY:N	2.66	0.44
1:B:332:GLN:N	1:B:332:GLN:OE1	2.40	0.44
1:B:446:PRO:HG2	1:B:447:ASN:H	1.81	0.43
1:A:291:VAL:O	1:A:293:ALA:N	2.51	0.43
1:A:440:PHE:CD2	1:A:453:ILE:HG22	2.53	0.43
1:A:515:PRO:HG2	1:A:516:ASN:N	2.24	0.43
1:B:366:LYS:HG2	1:B:367:ARG:N	2.24	0.43
1:B:289:ASN:CB	1:B:316:VAL:HG21	2.48	0.43
1:A:499:TRP:CG	1:A:505:PRO:HD3	2.53	0.43
1:B:220:GLY:O	1:B:222:TYR:N	2.50	0.43
1:B:187:PHE:CE2	1:B:189:ARG:HB3	2.54	0.43
1:A:459:PHE:HB2	1:A:461:ASP:OD2	2.18	0.43
1:A:310:VAL:HG11	1:A:471:LEU:HD21	2.01	0.43
1:A:310:VAL:HG21	1:A:471:LEU:CD2	2.48	0.43
1:A:310:VAL:CG1	1:A:317:ALA:HB3	2.44	0.43
1:A:150:TYR:HB2	1:A:153:VAL:HG12	2.00	0.43
1:A:208:PHE:O	1:A:210:TRP:N	2.51	0.43
1:A:269:ALA:HA	1:A:507:SER:OG	2.18	0.43
1:B:499:TRP:CG	1:B:505:PRO:HD3	2.53	0.43
1:A:178:LEU:O	1:A:181:LYS:NZ	2.51	0.43
1:B:47:ILE:HB	1:B:97:ASP:CG	2.39	0.43
1:B:434:TYR:O	1:B:437:LYS:HB2	2.19	0.43
1:B:473:GLN:HE21	1:B:476:GLY:N	2.17	0.43
1:B:174:THR:O	1:B:193:PRO:HA	2.19	0.43
1:A:540:LEU:CD1	1:A:559:LEU:HB3	2.49	0.43
1:A:362:SER:C	1:A:363:LEU:HD22	2.39	0.43
1:B:47:ILE:HD13	1:B:350:TRP:CE3	2.54	0.43
1:A:301:ASP:O	1:A:302:GLY:C	2.57	0.43
1:A:554:TRP:CD2	1:A:555:PRO:HD2	2.54	0.43
1:A:69:LEU:CD2	1:A:69:LEU:C	2.87	0.43
1:A:511:ASP:HB3	1:A:512:PRO:HD2	2.00	0.43
1:B:261:ARG:O	1:B:264:LEU:HB2	2.19	0.43
1:B:208:PHE:O	1:B:210:TRP:N	2.52	0.43
1:B:41:LEU:CD2	1:B:400:MET:HG2	2.47	0.43
1:B:469:PHE:HD2	1:B:480:TYR:HB3	1.84	0.43
1:A:196:TYR:CD1	1:A:196:TYR:N	2.86	0.43
1:B:359:PHE:O	1:B:360:GLN:HB2	2.19	0.42
1:A:418:LEU:HD22	1:A:422:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PHE:CD1	1:A:340:LEU:HD12	2.54	0.42
1:B:400:MET:O	1:B:403:ALA:HB3	2.19	0.42
1:A:443:PRO:C	1:A:445:ASN:H	2.21	0.42
1:A:93:VAL:HG23	1:A:95:ILE:HG13	2.00	0.42
1:A:157:VAL:HG12	1:A:161:LEU:CD2	2.49	0.42
1:B:389:LYS:O	1:B:392:PHE:N	2.52	0.42
1:B:59:ARG:NH1	1:B:59:ARG:CB	2.82	0.42
1:A:517:GLU:HG3	1:A:534:CYS:H	1.84	0.42
1:B:484:GLY:HA3	1:B:492:LEU:HA	2.00	0.42
1:A:97:ASP:OD1	1:A:98:THR:N	2.52	0.42
1:A:195:PHE:HD2	1:A:196:TYR:CE1	2.36	0.42
1:B:317:ALA:O	1:B:471:LEU:HD23	2.20	0.42
1:B:93:VAL:HG23	1:B:95:ILE:HG13	2.00	0.42
1:B:71:ALA:HA	1:B:333:PHE:CE1	2.55	0.42
1:B:473:GLN:NE2	1:B:476:GLY:N	2.64	0.42
1:A:196:TYR:HD1	1:A:196:TYR:N	2.18	0.42
1:B:187:PHE:CD2	1:B:188:ALA:N	2.88	0.42
1:A:167:PRO:HG3	1:A:430:LEU:HD23	2.01	0.42
1:A:513:CYS:HB3	1:A:518:MET:HB2	2.00	0.42
1:A:252:ILE:HG22	1:A:253:ARG:N	2.22	0.42
1:A:467:ASN:CB	1:A:469:PHE:HE1	2.33	0.42
1:B:219:GLU:HB2	1:B:247:VAL:O	2.19	0.42
1:B:303:TRP:CD1	1:B:322:THR:HG21	2.54	0.42
1:A:227:ILE:HD13	1:A:227:ILE:HA	1.82	0.42
1:A:107:GLU:O	1:A:110:LEU:HB2	2.19	0.42
1:B:400:MET:HA	1:B:400:MET:HE3	2.02	0.42
1:A:215:THR:HG22	1:A:273:VAL:HB	2.02	0.42
1:B:412:CYS:HA	1:B:413:PRO:HD2	1.66	0.42
1:A:426:ASP:HB3	1:A:429:LYS:HB2	2.02	0.42
1:B:399:ALA:O	1:B:400:MET:C	2.58	0.42
1:B:440:PHE:O	1:B:441:THR:C	2.56	0.42
1:B:443:PRO:C	1:B:445:ASN:H	2.22	0.42
1:B:341:ASN:OD1	1:B:344:ASN:ND2	2.53	0.42
1:A:218:SER:N	1:A:276:MET:HG2	2.35	0.41
1:A:407:MET:HG2	1:A:422:MET:SD	2.60	0.41
1:A:541:VAL:HG23	1:A:547:MET:CB	2.50	0.41
1:A:523:PRO:HG2	1:A:524:GLY:H	1.84	0.41
1:B:40:VAL:HG12	1:B:41:LEU:N	2.35	0.41
1:B:305:ALA:HA	1:B:480:TYR:CE2	2.55	0.41
1:B:215:THR:O	1:B:245:GLU:N	2.41	0.41
1:A:41:LEU:HD12	1:A:76:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:VAL:HG23	1:A:485:HIS:HA	2.02	0.41
1:B:356:GLU:OE1	1:B:363:LEU:HB2	2.21	0.41
1:B:205:LEU:HA	1:B:210:TRP:HE3	1.86	0.41
1:A:219:GLU:HB2	1:A:247:VAL:O	2.20	0.41
1:B:355:TRP:CE2	1:B:359:PHE:CE1	3.08	0.41
1:B:251:ASN:HD22	1:B:255:SER:HB3	1.85	0.41
1:A:486:TRP:O	1:A:486:TRP:HE3	2.03	0.41
1:A:67:GLN:HB3	1:A:390:ILE:HD11	2.02	0.41
1:B:40:VAL:HG21	1:B:140:LEU:HD22	2.02	0.41
1:B:459:PHE:HB2	1:B:461:ASP:OD2	2.21	0.41
1:A:305:ALA:HA	1:A:480:TYR:CD2	2.56	0.41
1:A:331:ARG:O	1:A:334:ASP:HB2	2.21	0.41
1:B:328:HIS:HA	1:B:329:PRO:HD2	1.87	0.41
1:A:213:VAL:HB	1:A:271:VAL:O	2.20	0.41
1:A:289:ASN:OD1	1:A:316:VAL:HG21	2.21	0.41
1:A:422:MET:O	1:A:423:LYS:C	2.57	0.41
1:B:426:ASP:O	1:B:427:GLY:C	2.57	0.41
1:B:435:LEU:O	1:B:437:LYS:N	2.51	0.41
1:A:310:VAL:HG13	1:A:317:ALA:CB	2.45	0.41
1:B:68:ARG:NH1	1:B:149:SER:OG	2.54	0.41
1:A:208:PHE:HB2	1:A:210:TRP:CE3	2.56	0.41
1:A:515:PRO:CG	1:A:516:ASN:N	2.84	0.41
1:A:289:ASN:HA	1:A:316:VAL:HG21	2.03	0.41
1:A:318:TYR:CG	1:A:319:GLY:N	2.89	0.41
1:A:356:GLU:OE1	1:A:363:LEU:HB2	2.20	0.40
1:A:215:THR:O	1:A:245:GLU:N	2.46	0.40
1:A:40:VAL:HA	1:A:92:GLY:O	2.21	0.40
1:A:214:SER:OG	1:A:243:THR:HG22	2.21	0.40
1:A:519:LYS:N	1:A:532:ILE:O	2.53	0.40
1:A:541:VAL:HG23	1:A:547:MET:HB2	2.02	0.40
1:A:85:LEU:O	1:A:86:LEU:C	2.59	0.40
1:B:301:ASP:O	1:B:304:GLY:N	2.54	0.40
1:A:504:VAL:HA	1:A:505:PRO:HD3	1.76	0.40
1:A:351:PHE:O	1:A:354:PHE:HB3	2.21	0.40
1:B:169:ILE:HG12	1:B:434:TYR:OH	2.22	0.40
1:A:341:ASN:ND2	1:A:341:ASN:O	2.54	0.40
1:B:399:ALA:HB1	1:B:434:TYR:HE1	1.85	0.40
1:A:341:ASN:OD1	1:A:344:ASN:ND2	2.54	0.40
1:B:215:THR:HG22	1:B:273:VAL:HB	2.03	0.40
1:B:181:LYS:CE	1:B:459:PHE:O	2.53	0.40
1:B:426:ASP:CG	1:B:429:LYS:HB2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:LYS:O	1:B:432:LYS:HG2	2.21	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	514/555 (93%)	415 (81%)	71 (14%)	28 (5%)	2	22
1	B	455/555 (82%)	368 (81%)	66 (14%)	21 (5%)	3	26
All	All	969/1110 (87%)	783 (81%)	137 (14%)	49 (5%)	2	24

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	ALA
1	A	292	ASN
1	A	361	CYS
1	A	443	PRO
1	A	494	VAL
1	A	518	MET
1	B	242	ALA
1	B	292	ASN
1	B	361	CYS
1	B	443	PRO
1	B	494	VAL
1	A	87	PRO
1	A	209	ASN
1	A	221	ASP
1	A	371	GLN
1	A	436	LEU
1	A	488	GLU

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Mol	Chain	Res	Type
1	A	495	ASP
1	A	516	ASN
1	A	523	PRO
1	A	566	PRO
1	B	87	PRO
1	B	100	SER
1	B	209	ASN
1	B	221	ASP
1	B	314	GLU
1	B	371	GLN
1	B	436	LEU
1	B	488	GLU
1	B	495	ASP
1	B	502	ASN
1	A	100	SER
1	A	314	GLU
1	A	450	ALA
1	A	502	ASN
1	B	441	THR
1	A	172	ALA
1	A	180	ASP
1	A	362	SER
1	A	492	LEU
1	A	536	PRO
1	B	180	ASP
1	B	362	SER
1	B	450	ALA
1	B	492	LEU
1	A	250	SER
1	A	446	PRO
1	B	446	PRO
1	A	267	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	447/481 (93%)	411 (92%)	36 (8%)	15	51
1	B	394/481 (82%)	368 (93%)	26 (7%)	21	61
All	All	841/962 (87%)	779 (93%)	62 (7%)	17	55

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	69	LEU
1	A	86	LEU
1	A	93	VAL
1	A	149	SER
1	A	153	VAL
1	A	161	LEU
1	A	174	THR
1	A	189	ARG
1	A	192	PRO
1	A	216	VAL
1	A	227	ILE
1	A	252	ILE
1	A	275	PHE
1	A	303	TRP
1	A	341	ASN
1	A	373	CYS
1	A	418	LEU
1	A	433	GLU
1	A	437	LYS
1	A	439	GLN
1	A	440	PHE
1	A	445	ASN
1	A	454	VAL
1	A	458	THR
1	A	461	ASP
1	A	492	LEU
1	A	498	HIS
1	A	502	ASN
1	A	504	VAL
1	A	518	MET
1	A	522	GLN
1	A	526	VAL
1	A	544	PHE
1	A	546	CYS

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Mol	Chain	Res	Type
1	A	548	ASP
1	B	67	GLN
1	B	86	LEU
1	B	93	VAL
1	B	149	SER
1	B	153	VAL
1	B	161	LEU
1	B	189	ARG
1	B	216	VAL
1	B	227	ILE
1	B	252	ILE
1	B	275	PHE
1	B	298	VAL
1	B	303	TRP
1	B	341	ASN
1	B	373	CYS
1	B	418	LEU
1	B	433	GLU
1	B	437	LYS
1	B	439	GLN
1	B	440	PHE
1	B	445	ASN
1	B	454	VAL
1	B	461	ASP
1	B	492	LEU
1	B	498	HIS
1	B	502	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	ASN
1	A	306	GLN
1	A	328	HIS
1	A	341	ASN
1	A	365	ASN
1	A	369	HIS
1	A	473	GLN
1	A	522	GLN
1	B	251	ASN
1	B	292	ASN
1	B	306	GLN

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Mol	Chain	Res	Type
1	B	328	HIS
1	B	341	ASN
1	B	344	ASN
1	B	365	ASN
1	B	369	HIS
1	B	473	GLN

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 ⓘ

3 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	$\# Z > 2$
3	52A	A	1001	-	4,12,12	0.81	0	4,18,18	1.13	0
2	NAG	A	801	1	14,14,15	0.77	1 (7%)	15,19,21	0.57	0
3	52A	B	2001	-	4,12,12	0.68	0	4,18,18	1.08	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	52A	A	1001	-	-	0/0/21/21	0/1/1/1
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	52A	B	2001	-	-	0/0/21/21	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAG	C1-C2	2.19	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	52A	2	0
3	B	2001	52A	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	518/555 (93%)	0.61	31 (5%)	25 23	38, 98, 201, 397	5 (0%)
1	B	459/555 (82%)	1.33	127 (27%)	1 1	52, 151, 269, 371	5 (1%)
All	All	977/1110 (88%)	0.95	158 (16%)	3 2	38, 117, 249, 397	10 (1%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	367	ARG	15.6
1	B	365	ASN	11.2
1	B	369	HIS	10.0
1	B	310	VAL	9.4
1	B	370	ARG	9.4
1	B	250	SER	8.2
1	B	321	ILE	7.7
1	B	323	LEU	7.1
1	B	364	GLN	6.6
1	A	365	ASN	6.6
1	A	366	LYS	6.1
1	B	298	VAL	6.0
1	B	274	LEU	5.8
1	B	254	LYS	5.8
1	B	210	TRP	5.7
1	B	443	PRO	5.6
1	B	284	LEU	5.6
1	B	272	VAL	5.3
1	B	303	TRP	5.2
1	B	297	TRP	5.2
1	B	204	ILE	4.8
1	B	322	THR	4.8
1	B	201	MET	4.7
1	B	471	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	271	VAL	4.7
1	B	273	VAL	4.6
1	B	62	GLU	4.6
1	B	371	GLN	4.5
1	B	200	ALA	4.5
1	B	492	LEU	4.5
1	B	379	ILE	4.4
1	B	483	VAL	4.4
1	B	299	ALA	4.2
1	B	213	VAL	4.1
1	B	198	ALA	4.1
1	B	434	TYR	4.1
1	B	233	GLU	4.0
1	B	469	PHE	4.0
1	B	307	GLU	4.0
1	B	72	MET	4.0
1	A	310	VAL	4.0
1	B	247	VAL	3.9
1	B	418	LEU	3.9
1	B	478	TYR	3.9
1	B	44	LEU	3.8
1	B	149	SER	3.8
1	B	368	ASN	3.8
1	B	497	ILE	3.8
1	A	414	GLN	3.7
1	B	486	TRP	3.7
1	B	171	TYR	3.7
1	B	251	ASN	3.7
1	B	494	VAL	3.6
1	B	389	LYS	3.5
1	B	320	ALA	3.5
1	B	480	TYR	3.5
1	B	390	ILE	3.5
1	B	350	TRP	3.4
1	A	66	ILE	3.4
1	B	355	TRP	3.4
1	B	173	SER	3.3
1	B	67	GLN	3.3
1	B	354	PHE	3.3
1	B	172	ALA	3.3
1	B	465	ARG	3.3
1	A	434	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	395	ASN	3.3
1	B	150	TYR	3.2
1	B	275	PHE	3.2
1	A	303	TRP	3.2
1	B	63	ASP	3.2
1	A	425	LEU	3.2
1	B	296	THR	3.2
1	A	247	VAL	3.1
1	B	456	PHE	3.1
1	B	214	SER	3.0
1	A	516	ASN	3.0
1	B	351	PHE	3.0
1	A	109	SER	3.0
1	A	520	ASN	3.0
1	B	340	LEU	3.0
1	B	46	PRO	2.9
1	B	317	ALA	2.9
1	B	205	LEU	2.9
1	B	398	TYR	2.9
1	B	490	LEU	2.9
1	A	494	VAL	2.9
1	B	109	SER	2.9
1	B	366	LYS	2.9
1	B	202	ALA	2.8
1	B	507	SER	2.8
1	B	68	ARG	2.8
1	B	248	GLY	2.8
1	B	253	ARG	2.8
1	B	96	LEU	2.8
1	B	216	VAL	2.8
1	B	95	ILE	2.8
1	A	471	LEU	2.7
1	B	363	LEU	2.7
1	B	199	LYS	2.7
1	B	396	ALA	2.7
1	B	337	PHE	2.7
1	B	241	ILE	2.7
1	B	263	LEU	2.7
1	B	333	PHE	2.7
1	B	66	ILE	2.7
1	B	285	ILE	2.7
1	B	86	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	95	ILE	2.6
1	B	470	ASN	2.6
1	B	89	VAL	2.6
1	B	190	THR	2.6
1	B	237	ARG	2.6
1	B	156	GLN	2.6
1	B	336	TYR	2.6
1	A	91	LEU	2.5
1	B	384	TYR	2.5
1	B	499	TRP	2.5
1	B	359	PHE	2.5
1	A	323	LEU	2.4
1	B	325	LEU	2.4
1	B	468	VAL	2.4
1	B	39	LEU	2.4
1	B	249	ARG	2.4
1	A	499	TRP	2.4
1	A	178	LEU	2.3
1	B	281	SER	2.3
1	B	309	ILE	2.3
1	A	454	VAL	2.3
1	B	372	VAL	2.3
1	B	197	GLN	2.3
1	B	264	LEU	2.3
1	B	300	SER	2.3
1	B	444	PHE	2.2
1	B	208	PHE	2.2
1	A	317	ALA	2.2
1	B	222	TYR	2.2
1	B	84	TYR	2.2
1	B	212	TYR	2.2
1	B	79	ILE	2.2
1	A	251	ASN	2.2
1	A	89	VAL	2.1
1	B	41	LEU	2.1
1	A	517	GLU	2.1
1	B	91	LEU	2.1
1	B	446	PRO	2.1
1	A	79	ILE	2.1
1	A	200	ALA	2.1
1	A	390	ILE	2.1
1	B	160	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	156	GLN	2.0
1	B	148	GLY	2.0
1	B	464	GLY	2.0
1	A	93	VAL	2.0
1	B	311	LYS	2.0
1	B	207	PHE	2.0
1	B	194	ASP	2.0
1	A	175	SER	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(\AA^2)	Q<0.9
3	52A	B	2001	12/12	0.93	0.59	1.05	94,94,94,94	0
3	52A	A	1001	12/12	0.97	0.33	0.72	64,64,64,64	0
2	NAG	A	801	14/15	0.63	0.43	-	210,210,210,210	0

6.5 Other polymers [i](#)

There are no such residues in this entry.