



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:49 PM UTC

PDB ID : 4YG8 / pdb_00004yg8
Title : CRYSTAL STRUCTURE OF THE CHS5-CHS6 EXOMER CARGO ADAPTOR COMPLEX
Authors : Paczkowski, J.E.; Richardson, B.C.; Strassner, A.M.; Fromme, J.C.
Deposited on : 2015-02-26
Resolution : 2.75 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

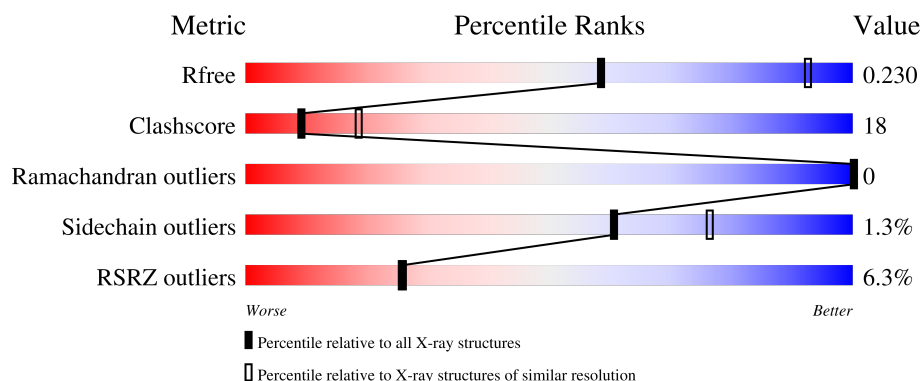
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	290	9% 61% 33% • 5%
2	B	754	4% 66% 21% • 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7752 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 Chitin biosynthesis protein CHS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2082	1316	365	393	8			

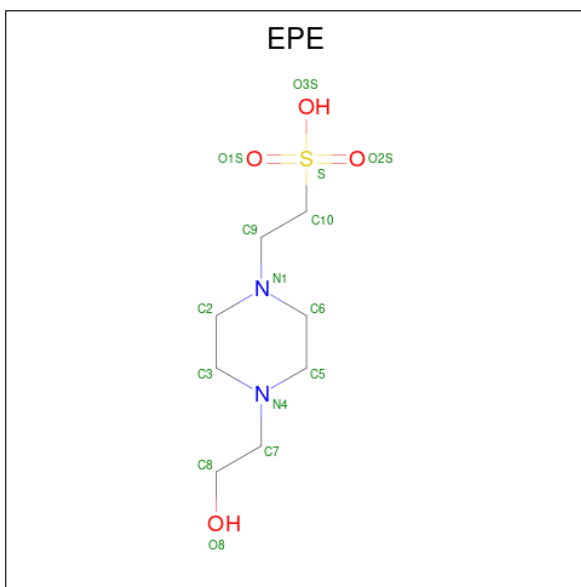
- Molecule 2 is a protein called Chitin biosynthesis protein CHS6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	673	Total	C	N	O	S	0	0	0
			5446	3495	897	1015	39			

There are 8 discrepancies between the modelled and reference sequences:

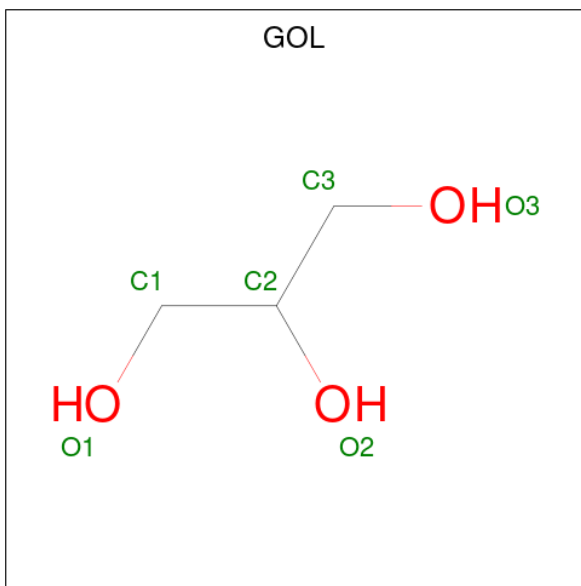
Chain	Residue	Modelled	Actual	Comment	Reference
B	747	GLY	-	expression tag	UNP P40955
B	748	THR	-	expression tag	UNP P40955
B	749	GLU	-	expression tag	UNP P40955
B	750	ASN	-	expression tag	UNP P40955
B	751	LEU	-	expression tag	UNP P40955
B	752	TYR	-	expression tag	UNP P40955
B	753	PHE	-	expression tag	UNP P40955
B	754	GLN	-	expression tag	UNP P40955

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

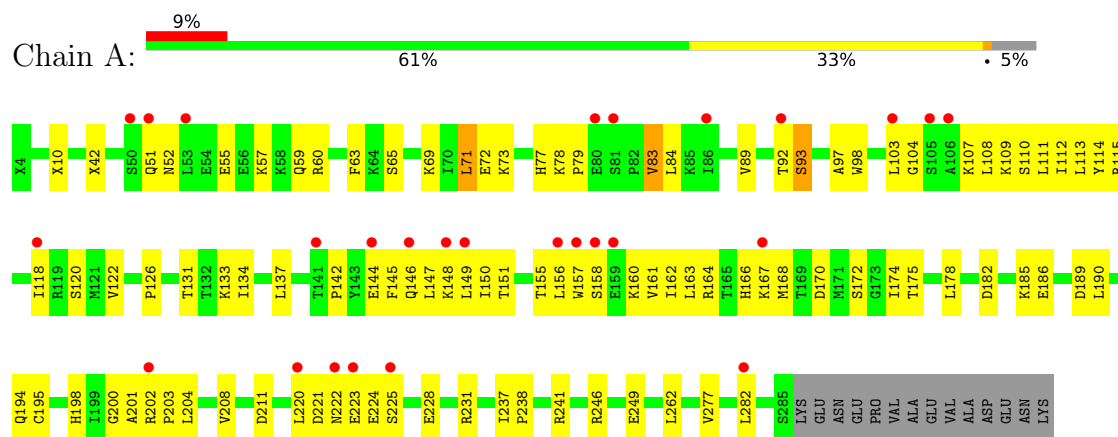
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total 39	O 39	0	0
5	B	164	Total 164	O 164	0	0

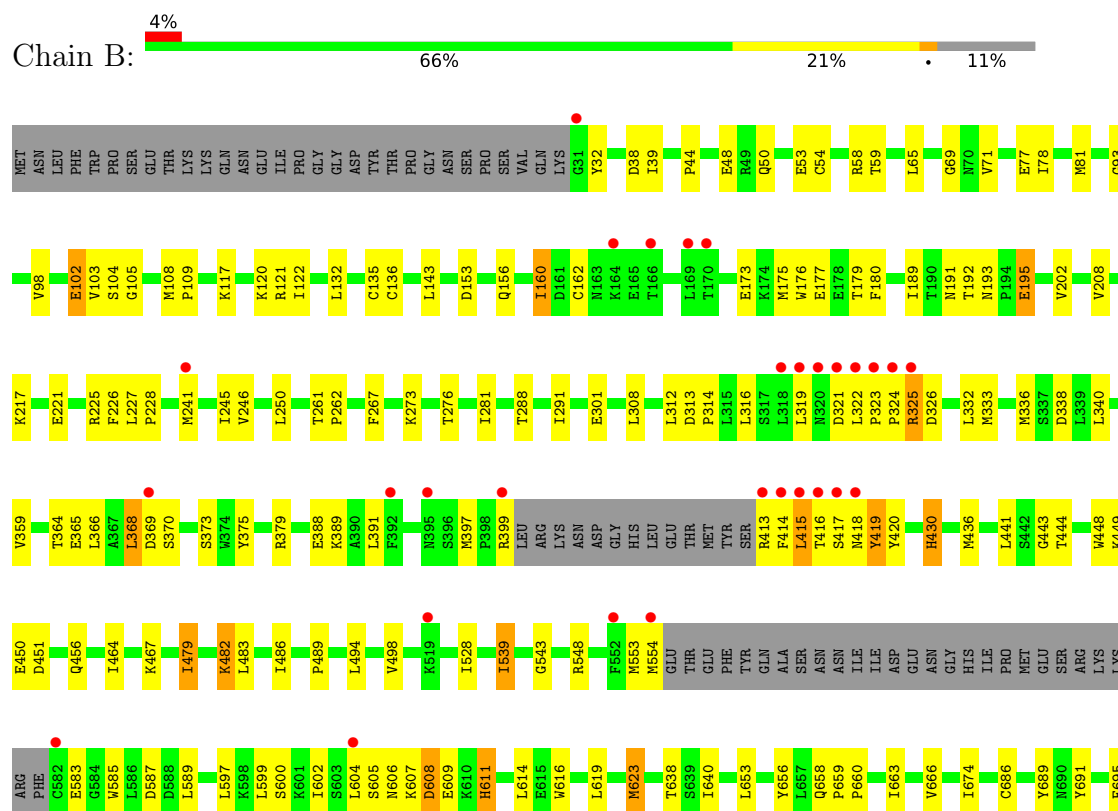
3 Residue-property plots [i](#)

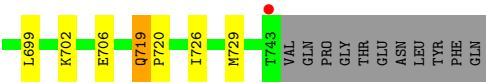
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Chitin biosynthesis protein CHS5



• Molecule 2: Chitin biosynthesis protein CHS6





4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	165.75Å 165.75Å 263.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.07 – 2.75 47.07 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.07-2.75) 90.8 (47.07-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 2.73Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.193 , 0.230 0.196 , 0.230	Depositor DCC
R_{free} test set	2856 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7752	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, EPE

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	0.63	1/1919 (0.1%)	0.96	7/2599 (0.3%)
2	B	0.60	2/5555 (0.0%)	0.91	21/7516 (0.3%)
All	All	0.61	3/7474 (0.0%)	0.92	28/10115 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	156	GLN	CD-OE1	5.51	1.34	1.23
1	A	51	GLN	CD-OE1	5.13	1.33	1.23
2	B	611	HIS	ND1-CE1	5.04	1.37	1.32

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	312	LEU	N-CA-C	9.51	121.72	111.36
1	A	107	LYS	N-CA-C	-7.49	99.94	110.50
2	B	482	LYS	N-CA-C	-7.44	100.51	110.55
2	B	419	TYR	N-CA-C	6.61	119.31	111.71
2	B	611	HIS	CB-CG-CD2	-6.55	122.68	131.20
2	B	397	MET	N-CA-C	6.46	118.82	109.84
2	B	658	GLN	CA-C-N	5.86	123.88	119.66
2	B	658	GLN	C-N-CA	5.86	123.88	119.66
2	B	417	SER	N-CA-C	5.85	119.39	112.72
1	A	186	GLU	N-CA-C	5.69	119.42	111.74
2	B	611	HIS	CB-CG-ND1	5.64	131.16	122.70
2	B	420	TYR	N-CA-C	5.61	118.62	109.59
2	B	608	ASP	N-CA-C	-5.54	105.15	112.24
1	A	93	SER	N-CA-C	5.51	117.17	108.96
2	B	479	ILE	N-CA-C	5.51	116.24	110.62
2	B	102	GLU	N-CA-C	5.47	116.94	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	LEU	CA-C-N	-5.45	113.36	120.44
1	A	71	LEU	C-N-CA	-5.45	113.36	120.44
1	A	73	LYS	N-CA-C	5.32	117.08	111.28
1	A	158	SER	N-CA-C	5.12	115.10	107.88
2	B	368	LEU	N-CA-C	-5.11	107.04	113.28
2	B	719	GLN	CA-C-N	5.10	124.89	119.28
2	B	719	GLN	C-N-CA	5.10	124.89	119.28
2	B	69	GLY	N-CA-C	5.08	118.83	112.73
2	B	659	PRO	O-C-N	5.08	123.54	121.15
2	B	450	GLU	N-CA-C	5.08	116.81	111.28
2	B	539	ILE	N-CA-C	5.07	117.85	112.83
2	B	325	ARG	N-CA-C	-5.04	107.08	113.23

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	2082	0	1975	126	0
2	B	5446	0	5494	151	1
3	B	15	0	17	4	0
4	B	6	0	8	0	0
5	A	39	0	0	0	0
5	B	164	0	0	4	0
All	All	7752	0	7494	274	1

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 18.

All (274) 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)
2:B:323:PRO:CD	2:B:324:PRO:HD3	1.37	1.52
1:A:221:ASP:O	1:A:222:ASN:CG	1.84	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:O	1:A:223:GLU:HB3	1.44	1.16
2:B:323:PRO:HD2	2:B:324:PRO:CD	1.76	1.15
2:B:323:PRO:CD	2:B:324:PRO:CD	2.30	1.09
1:A:220:LEU:HD21	1:A:262:LEU:HD22	1.43	0.99
1:A:112:ILE:HG12	1:A:122:VAL:HG22	1.47	0.97
2:B:241:MET:SD	2:B:369:ASP:O	2.24	0.95
2:B:323:PRO:N	2:B:324:PRO:CD	2.30	0.93
2:B:192:THR:HA	3:B:801:EPE:H31	1.51	0.92
2:B:103:VAL:HG12	2:B:103:VAL:O	1.70	0.91
1:A:103:LEU:HD21	1:A:151:THR:HG21	1.51	0.90
2:B:436:MET:HE2	2:B:436:MET:HA	1.52	0.90
1:A:97:ALA:HB2	1:A:131:THR:HG22	1.51	0.90
1:A:109:LYS:HB2	1:A:150:ILE:HG22	1.51	0.90
1:A:246:ARG:NH1	1:A:249:GLU:OE1	2.04	0.90
2:B:323:PRO:N	2:B:324:PRO:HD3	1.84	0.88
1:A:79:PRO:HB3	1:A:103:LEU:CD2	2.04	0.87
2:B:323:PRO:HD2	2:B:324:PRO:HD3	0.86	0.85
1:A:148:LYS:HA	1:A:157:TRP:HB3	1.57	0.85
1:A:108:LEU:CD1	1:A:149:LEU:HD11	2.06	0.84
1:A:79:PRO:HB3	1:A:103:LEU:HD23	1.59	0.84
2:B:663:ILE:CG2	2:B:666:VAL:HB	2.08	0.84
1:A:111:LEU:CD2	1:A:126:PRO:HB3	2.09	0.82
1:A:103:LEU:CD2	1:A:151:THR:HG21	2.10	0.81
1:A:144:GLU:HB3	1:A:162:ILE:HG22	1.62	0.80
1:A:79:PRO:CB	1:A:103:LEU:HD23	2.11	0.80
1:A:146:GLN:HB3	1:A:160:LYS:HB3	1.62	0.80
1:A:202:ARG:HG3	1:A:203:PRO:HD2	1.63	0.79
1:A:220:LEU:O	1:A:223:GLU:CB	2.30	0.78
1:A:221:ASP:O	1:A:222:ASN:OD1	2.00	0.78
2:B:660:PRO:HD2	2:B:663:ILE:HD12	1.65	0.78
1:A:110:SER:HB3	1:A:150:ILE:HB	1.66	0.77
2:B:597:LEU:O	2:B:600:SER:OG	2.02	0.77
1:A:59:GLN:OE1	1:A:59:GLN:HA	1.85	0.76
2:B:250:LEU:HD23	2:B:250:LEU:C	2.11	0.76
2:B:301:GLU:OE2	5:B:964:HOH:O	2.05	0.75
1:A:202:ARG:CG	1:A:203:PRO:HD2	2.16	0.75
2:B:604:LEU:CD1	2:B:619:LEU:HD22	2.17	0.75
1:A:220:LEU:HD21	1:A:262:LEU:CD2	2.16	0.75
1:A:220:LEU:HG	1:A:262:LEU:HD23	1.68	0.74
1:A:111:LEU:HD23	1:A:126:PRO:HB3	1.69	0.74
2:B:53:GLU:HG3	2:B:54:CYS:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:HD22	1:A:204:LEU:HD21	1.72	0.72
1:A:175:THR:HG22	1:A:202:ARG:HB3	1.71	0.71
1:A:113:LEU:O	1:A:120:SER:HB2	1.89	0.71
1:A:118:ILE:HG12	1:A:118:ILE:O	1.88	0.71
2:B:117:LYS:NZ	2:B:153:ASP:OD1	2.22	0.71
1:A:108:LEU:HD11	1:A:149:LEU:CD1	2.19	0.70
2:B:619:LEU:HG	2:B:623:MET:CE	2.20	0.70
1:A:79:PRO:CB	1:A:103:LEU:CD2	2.69	0.70
2:B:498:VAL:HG21	2:B:614:LEU:HD22	1.73	0.70
1:A:55:GLU:OE2	1:A:55:GLU:HA	1.91	0.70
2:B:217:LYS:HE2	2:B:267:PHE:CE1	2.27	0.69
2:B:323:PRO:CG	2:B:324:PRO:HD3	2.19	0.69
1:A:178:LEU:HB2	1:A:204:LEU:HD11	1.74	0.69
2:B:103:VAL:O	2:B:103:VAL:CG1	2.41	0.68
1:A:108:LEU:HD11	1:A:149:LEU:HD11	1.75	0.68
1:A:111:LEU:HD22	1:A:126:PRO:HB3	1.75	0.68
2:B:663:ILE:HG21	2:B:666:VAL:HB	1.75	0.68
1:A:144:GLU:CB	1:A:162:ILE:HG22	2.24	0.68
1:A:148:LYS:HG3	1:A:157:TRP:CD1	2.28	0.67
2:B:364:THR:O	2:B:368:LEU:HD23	1.94	0.67
2:B:413:ARG:HG3	2:B:414:PHE:HD1	1.60	0.67
1:A:108:LEU:HD13	1:A:149:LEU:HD11	1.75	0.67
2:B:177:GLU:HG2	2:B:226:PHE:HE1	1.60	0.65
1:A:103:LEU:CD1	1:A:108:LEU:HB2	2.25	0.65
1:A:148:LYS:HG3	1:A:157:TRP:HD1	1.60	0.65
2:B:366:LEU:HD12	5:B:910:HOH:O	1.95	0.65
1:A:72:GLU:OE2	1:A:78:LYS:NZ	2.20	0.64
1:A:103:LEU:HD11	1:A:108:LEU:HB2	1.79	0.64
1:A:147:LEU:O	1:A:157:TRP:HB2	1.98	0.64
1:A:89:VAL:HG12	1:A:166:HIS:HD2	1.62	0.64
1:A:221:ASP:O	1:A:222:ASN:ND2	2.30	0.64
1:A:161:VAL:HG12	1:A:162:ILE:N	2.13	0.63
2:B:605:SER:O	2:B:606:ASN:HB2	1.98	0.63
1:A:146:GLN:HB3	1:A:160:LYS:CB	2.27	0.62
2:B:340:LEU:HD22	2:B:359:VAL:HG13	1.80	0.62
2:B:553:MET:O	2:B:554:MET:HB2	1.99	0.62
1:A:208:VAL:N	1:A:228:GLU:OE1	2.31	0.62
1:A:89:VAL:O	1:A:166:HIS:CD2	2.53	0.62
1:A:133:LYS:C	1:A:134:ILE:HD13	2.24	0.61
1:A:65:SER:O	1:A:69:LYS:HG3	2.00	0.61
2:B:81:MET:HG2	2:B:132:LEU:CD2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:619:LEU:HG	2:B:623:MET:HE1	1.83	0.61
2:B:177:GLU:HG2	2:B:226:PHE:CE1	2.36	0.61
2:B:399:ARG:HD3	2:B:585:TRP:CD1	2.36	0.61
1:A:149:LEU:O	1:A:155:THR:HA	2.01	0.60
1:A:163:LEU:HD12	1:A:163:LEU:O	2.01	0.60
2:B:482:LYS:O	2:B:483:LEU:HB2	2.01	0.60
1:A:108:LEU:CD1	1:A:149:LEU:CD1	2.78	0.60
2:B:58:ARG:HD2	2:B:78:ILE:CD1	2.31	0.60
2:B:102:GLU:OE2	2:B:102:GLU:HA	2.02	0.60
2:B:656:TYR:CE2	2:B:702:LYS:HD3	2.36	0.60
1:A:220:LEU:CD2	1:A:262:LEU:CD2	2.80	0.59
2:B:44:PRO:HD3	2:B:689:TYR:CE1	2.37	0.59
1:A:220:LEU:CG	1:A:262:LEU:HD23	2.32	0.59
1:A:79:PRO:HB3	1:A:103:LEU:HD22	1.81	0.59
1:A:92:THR:HG22	1:A:92:THR:O	2.01	0.59
1:A:224:GLU:O	1:A:225:SER:CB	2.49	0.59
2:B:418:ASN:OD1	2:B:419:TYR:N	2.36	0.58
2:B:695:PHE:HB2	3:B:801:EPE:H82	1.85	0.58
2:B:44:PRO:HD3	2:B:689:TYR:CZ	2.39	0.58
2:B:365:GLU:HB3	5:B:910:HOH:O	2.03	0.58
2:B:413:ARG:HG3	2:B:414:PHE:CD1	2.38	0.58
1:A:93:SER:HA	1:A:137:LEU:HD12	1.86	0.57
1:A:142:PRO:HG3	1:A:164:ARG:HG2	1.87	0.57
2:B:81:MET:HG2	2:B:132:LEU:HD22	1.85	0.57
1:A:60:ARG:HG2	2:B:316:LEU:HD21	1.87	0.57
1:A:221:ASP:C	1:A:222:ASN:CG	2.71	0.57
2:B:528:ILE:HD13	2:B:585:TRP:HZ3	1.68	0.57
2:B:375:TYR:CE1	2:B:379:ARG:HD2	2.40	0.57
1:A:108:LEU:HD12	1:A:151:THR:HG22	1.85	0.56
2:B:103:VAL:HG11	2:B:179:THR:HG22	1.86	0.56
2:B:441:LEU:O	2:B:444:THR:OG1	2.23	0.56
2:B:322:LEU:HB3	2:B:324:PRO:HD2	1.87	0.56
1:A:79:PRO:HB3	1:A:103:LEU:HA	1.86	0.56
2:B:59:THR:HG23	2:B:162:CYS:SG	2.45	0.56
1:A:149:LEU:HB3	1:A:156:LEU:O	2.06	0.56
2:B:599:LEU:HD23	2:B:602:ILE:HD11	1.88	0.56
2:B:48:GLU:HG2	2:B:53:GLU:HG2	1.88	0.55
2:B:528:ILE:HD13	2:B:585:TRP:CZ3	2.41	0.55
1:A:52:ASN:ND2	1:A:55:GLU:HB2	2.20	0.55
1:A:109:LYS:HB2	1:A:150:ILE:CG2	2.33	0.55
1:A:223:GLU:CG	1:A:224:GLU:N	2.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:GLU:HG2	2:B:489:PRO:HA	1.88	0.55
1:A:108:LEU:CD1	1:A:151:THR:HG22	2.37	0.55
2:B:217:LYS:HG2	2:B:267:PHE:CE2	2.42	0.55
1:A:89:VAL:HG12	1:A:166:HIS:CD2	2.42	0.55
1:A:161:VAL:CG1	1:A:162:ILE:N	2.69	0.55
2:B:160:ILE:N	2:B:160:ILE:HD13	2.22	0.55
1:A:92:THR:O	1:A:137:LEU:HB2	2.08	0.54
1:A:10:UNK:O	1:A:42:UNK:N	2.40	0.54
1:A:84:LEU:HD13	1:A:147:LEU:HG	1.88	0.54
2:B:217:LYS:HE2	2:B:267:PHE:CD1	2.42	0.54
1:A:220:LEU:O	1:A:223:GLU:N	2.41	0.54
1:A:189:ASP:OD1	1:A:190:LEU:N	2.41	0.53
1:A:112:ILE:CG1	1:A:122:VAL:HG22	2.30	0.53
2:B:325:ARG:HG2	2:B:325:ARG:O	2.08	0.53
1:A:79:PRO:HB2	1:A:103:LEU:HD23	1.91	0.52
1:A:71:LEU:O	1:A:72:GLU:C	2.50	0.52
2:B:313:ASP:HB2	2:B:314:PRO:HD3	1.92	0.52
2:B:619:LEU:HG	2:B:623:MET:HE3	1.90	0.52
2:B:663:ILE:HG22	2:B:666:VAL:H	1.73	0.52
2:B:324:PRO:O	2:B:325:ARG:HB3	2.10	0.52
2:B:663:ILE:HG23	2:B:666:VAL:HB	1.92	0.52
2:B:246:VAL:HG21	2:B:338:ASP:HB3	1.92	0.52
2:B:599:LEU:HD23	2:B:602:ILE:CD1	2.39	0.52
1:A:118:ILE:O	1:A:118:ILE:CG1	2.59	0.51
2:B:105:GLY:HA2	2:B:176:TRP:CE3	2.46	0.51
2:B:604:LEU:HD11	2:B:619:LEU:HD22	1.91	0.51
1:A:223:GLU:HG3	1:A:224:GLU:N	2.25	0.51
2:B:191:ASN:O	3:B:801:EPE:C2	2.59	0.51
2:B:273:LYS:O	2:B:276:THR:HG22	2.10	0.51
1:A:190:LEU:HD11	1:A:282:LEU:HD13	1.93	0.51
1:A:208:VAL:HG23	1:A:228:GLU:OE1	2.10	0.50
1:A:147:LEU:O	1:A:157:TRP:CB	2.59	0.50
2:B:250:LEU:C	2:B:250:LEU:CD2	2.83	0.50
2:B:58:ARG:HD2	2:B:78:ILE:HD11	1.93	0.50
1:A:108:LEU:HD11	1:A:149:LEU:HD12	1.93	0.50
1:A:114:TYR:CE2	1:A:118:ILE:HB	2.46	0.50
2:B:143:LEU:CD1	2:B:175:MET:HE3	2.42	0.50
1:A:77:HIS:HB3	1:A:104:GLY:HA3	1.94	0.50
2:B:479:ILE:O	2:B:482:LYS:O	2.30	0.49
1:A:221:ASP:O	1:A:222:ASN:CB	2.56	0.49
1:A:167:LYS:HG2	1:A:168:MET:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:LEU:HD23	2:B:250:LEU:O	2.12	0.49
2:B:81:MET:HA	2:B:132:LEU:HD23	1.95	0.49
2:B:607:LYS:O	2:B:608:ASP:HB2	2.10	0.49
2:B:217:LYS:HG2	2:B:267:PHE:CZ	2.48	0.48
1:A:149:LEU:HG	1:A:151:THR:HG23	1.94	0.48
2:B:245:ILE:HG22	2:B:288:THR:HG21	1.94	0.48
2:B:604:LEU:HG	2:B:619:LEU:HD22	1.95	0.48
2:B:660:PRO:CD	2:B:663:ILE:HD12	2.38	0.48
2:B:191:ASN:O	3:B:801:EPE:H22	2.12	0.48
2:B:415:LEU:HG	2:B:415:LEU:O	2.14	0.48
2:B:122:ILE:HA	2:B:443:GLY:O	2.13	0.48
2:B:58:ARG:HD2	2:B:78:ILE:HD13	1.95	0.48
1:A:134:ILE:HD13	1:A:134:ILE:N	2.28	0.47
2:B:430:HIS:CD2	2:B:430:HIS:N	2.81	0.47
2:B:77:GLU:HG3	2:B:136:CYS:HA	1.96	0.47
1:A:115:ARG:HB2	1:A:144:GLU:O	2.14	0.47
2:B:189:ILE:O	2:B:193:ASN:ND2	2.40	0.47
2:B:120:LYS:O	2:B:121:ARG:HD3	2.15	0.47
1:A:162:ILE:HG13	1:A:162:ILE:O	2.13	0.47
2:B:449:LYS:HG2	2:B:451:ASP:OD1	2.15	0.47
1:A:194:GLN:O	1:A:198:HIS:ND1	2.48	0.47
2:B:32:TYR:HB2	2:B:208:VAL:CG1	2.45	0.47
1:A:175:THR:HG22	1:A:202:ARG:CB	2.44	0.47
1:A:224:GLU:O	1:A:225:SER:OG	2.30	0.47
1:A:60:ARG:HG2	2:B:316:LEU:CD2	2.44	0.47
1:A:182:ASP:HB3	1:A:185:LYS:HD2	1.96	0.47
1:A:202:ARG:NH1	1:A:211:ASP:OD2	2.47	0.47
2:B:44:PRO:HB3	2:B:689:TYR:OH	2.15	0.47
2:B:663:ILE:CG2	2:B:666:VAL:CB	2.88	0.47
2:B:604:LEU:HD22	2:B:611:HIS:CE1	2.50	0.46
2:B:464:ILE:O	2:B:464:ILE:HG13	2.14	0.46
2:B:291:ILE:HD13	2:B:308:LEU:HD23	1.97	0.46
2:B:415:LEU:HD12	2:B:415:LEU:C	2.40	0.46
1:A:57:LYS:HA	1:A:60:ARG:NH2	2.30	0.46
1:A:92:THR:O	1:A:92:THR:CG2	2.64	0.46
2:B:482:LYS:O	2:B:483:LEU:CB	2.63	0.46
1:A:195:CYS:HA	1:A:198:HIS:ND1	2.31	0.45
2:B:48:GLU:OE2	2:B:93:GLY:HA3	2.16	0.45
2:B:103:VAL:HG11	2:B:179:THR:CG2	2.47	0.45
2:B:430:HIS:CD2	2:B:430:HIS:H	2.34	0.45
1:A:172:SER:HA	1:A:200:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:GLU:HB3	2:B:225:ARG:NH1	2.31	0.45
2:B:695:PHE:CE2	2:B:699:LEU:HD11	2.51	0.45
2:B:319:LEU:HD13	2:B:333:MET:HG3	1.99	0.45
2:B:616:TRP:CE2	2:B:638:THR:HG21	2.52	0.45
1:A:167:LYS:HG2	1:A:168:MET:H	1.82	0.45
1:A:202:ARG:HG2	1:A:203:PRO:HD2	1.98	0.45
2:B:227:LEU:N	2:B:228:PRO:CD	2.80	0.45
2:B:604:LEU:HD22	2:B:611:HIS:ND1	2.33	0.44
2:B:103:VAL:CG1	2:B:179:THR:HG22	2.48	0.44
1:A:190:LEU:HD23	1:A:277:VAL:HG11	2.00	0.44
1:A:208:VAL:HB	1:A:231:ARG:HD2	2.00	0.44
2:B:388:GLU:OE1	2:B:388:GLU:N	2.43	0.44
2:B:494:LEU:HB3	2:B:498:VAL:HG13	1.99	0.44
2:B:548:ARG:NH1	2:B:587:ASP:OD1	2.51	0.44
2:B:604:LEU:CG	2:B:619:LEU:HD22	2.48	0.44
1:A:114:TYR:HB2	1:A:146:GLN:HG3	2.00	0.44
2:B:619:LEU:HD12	2:B:619:LEU:HA	1.71	0.44
2:B:436:MET:HA	2:B:436:MET:CE	2.37	0.44
2:B:103:VAL:HG22	2:B:109:PRO:HG2	2.01	0.43
1:A:103:LEU:HD22	1:A:151:THR:HG21	1.96	0.43
1:A:237:ILE:HG23	1:A:238:PRO:HD2	2.00	0.43
2:B:416:THR:O	2:B:419:TYR:CE2	2.71	0.43
2:B:322:LEU:C	2:B:324:PRO:HD2	2.44	0.43
2:B:539:ILE:HG13	2:B:543:GLY:HA3	1.99	0.43
2:B:322:LEU:C	2:B:324:PRO:CD	2.92	0.43
2:B:686:CYS:SG	2:B:729:MET:HG2	2.59	0.43
2:B:38:ASP:OD1	2:B:467:LYS:HG3	2.19	0.43
2:B:173:GLU:OE1	2:B:173:GLU:HA	2.19	0.43
1:A:79:PRO:HB2	1:A:103:LEU:CD2	2.49	0.42
2:B:261:THR:N	2:B:262:PRO:CD	2.82	0.42
2:B:370:SER:HB3	2:B:373:SER:HB2	2.01	0.42
2:B:48:GLU:HG2	2:B:53:GLU:CG	2.48	0.42
2:B:108:MET:HB2	2:B:109:PRO:HD3	2.01	0.42
2:B:98:VAL:HA	2:B:202:VAL:O	2.20	0.42
2:B:104:SER:HA	2:B:180:PHE:HB2	2.02	0.42
2:B:323:PRO:N	2:B:324:PRO:HD2	2.30	0.42
2:B:326:ASP:OD1	2:B:326:ASP:N	2.52	0.42
1:A:113:LEU:C	1:A:120:SER:HB2	2.45	0.42
2:B:39:ILE:HG12	2:B:691:TYR:CD2	2.54	0.42
2:B:103:VAL:HG22	2:B:109:PRO:CG	2.50	0.42
2:B:640:ILE:HG22	2:B:640:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:HIS:HD1	1:A:170:ASP:CG	2.25	0.42
1:A:241:ARG:NH2	1:A:262:LEU:O	2.53	0.41
2:B:583:GLU:HB3	2:B:585:TRP:CD1	2.55	0.41
1:A:133:LYS:O	1:A:134:ILE:HD13	2.20	0.41
2:B:389:LYS:HG3	5:B:942:HOH:O	2.19	0.41
2:B:653:LEU:HB3	2:B:699:LEU:HD11	2.01	0.41
1:A:222:ASN:OD1	1:A:222:ASN:C	2.64	0.41
2:B:65:LEU:HB3	2:B:71:VAL:HA	2.03	0.41
2:B:391:LEU:HD12	2:B:391:LEU:HA	1.82	0.41
1:A:79:PRO:CB	1:A:103:LEU:HD22	2.44	0.41
1:A:174:ILE:O	1:A:201:ALA:HB1	2.21	0.41
1:A:118:ILE:O	1:A:120:SER:O	2.39	0.41
1:A:163:LEU:HD12	1:A:163:LEU:C	2.46	0.41
2:B:53:GLU:HG3	2:B:54:CYS:H	1.83	0.41
2:B:78:ILE:HG12	2:B:135:CYS:HB2	2.03	0.41
2:B:448:TRP:CZ2	2:B:464:ILE:HB	2.56	0.41
2:B:702:LYS:O	2:B:706:GLU:HG3	2.21	0.41
1:A:113:LEU:HD11	1:A:145:PHE:HB3	2.01	0.41
2:B:607:LYS:HB3	2:B:609:GLU:HG3	2.03	0.40
2:B:674:ILE:HD13	2:B:674:ILE:HA	1.95	0.40
2:B:719:GLN:HA	2:B:720:PRO:HD2	1.89	0.40
1:A:63:PHE:CD2	2:B:316:LEU:HD22	2.56	0.40
1:A:144:GLU:HA	1:A:161:VAL:O	2.21	0.40
2:B:316:LEU:HA	2:B:336:MET:HE1	2.03	0.40
2:B:589:LEU:HD23	2:B:589:LEU:HA	1.90	0.40
1:A:83:VAL:O	1:A:98:TRP:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:GLN:NE2	2:B:321:ASP:OD2[2_445]	2.17	0.03

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	234/290 (81%)	226 (97%)	8 (3%)	0	100	100
2	B	667/754 (88%)	651 (98%)	16 (2%)	0	100	100
All	All	901/1044 (86%)	877 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	218/230 (95%)	217 (100%)	1 (0%)	81	89
2	B	616/690 (89%)	606 (98%)	10 (2%)	55	73
All	All	834/920 (91%)	823 (99%)	11 (1%)	61	76

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	VAL
2	B	160	ILE
2	B	195	GLU
2	B	281	ILE
2	B	332	LEU
2	B	415	LEU
2	B	430	HIS
2	B	456	GLN
2	B	486	ILE
2	B	623	MET
2	B	726	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	226	ASN
2	B	56	HIS
2	B	247	ASN
2	B	343	GLN
2	B	349	ASN
2	B	501	GLN
2	B	651	GLN
2	B	710	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
4	GOL	B	802	-	5,5,5	0.32	0	5,5,5	0.73	0
3	EPE	B	801	-	15,15,15	0.89	1 (6%)	19,20,20	1.25	2 (10%)

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
4	GOL	B	802	-	-	4/4/4/4	-
3	EPE	B	801	-	-	4/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	EPE	C10-S	2.99	1.81	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	EPE	C6-N1-C2	2.26	113.70	108.84
3	B	801	EPE	O3S-S-C10	2.00	109.92	106.00

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	EPE	C8-C7-N4-C3
4	B	802	GOL	C1-C2-C3-O3
4	B	802	GOL	O1-C1-C2-C3
3	B	801	EPE	C10-C9-N1-C2
4	B	802	GOL	O2-C2-C3-O3
3	B	801	EPE	C8-C7-N4-C5
3	B	801	EPE	C10-C9-N1-C6
4	B	802	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	EPE	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	48:UNK	C	50:SER	N	3.76
1	A	12:UNK	C	18:UNK	N	3.05

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	236/290 (81%)	0.53	27 (11%) 10 8	35, 83, 150, 175	0
2	B	673/754 (89%)	-0.24	30 (4%) 38 37	24, 49, 109, 182	0
All	All	909/1044 (87%)	-0.04	57 (6%) 26 26	24, 55, 129, 182	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	322	LEU	5.7
2	B	416	THR	5.6
1	A	156	LEU	5.4
2	B	415	LEU	5.0
2	B	395	ASN	4.8
2	B	552	PHE	4.7
1	A	146	GLN	4.5
1	A	51	GLN	4.4
2	B	31	GLY	4.1
2	B	369	ASP	4.0
1	A	167	LYS	4.0
2	B	325	ARG	3.9
1	A	53	LEU	3.8
1	A	202	ARG	3.6
2	B	166	THR	3.6
2	B	164	LYS	3.6
2	B	417	SER	3.6
1	A	106	ALA	3.5
1	A	157	TRP	3.4
1	A	103	LEU	3.3
1	A	222	ASN	3.1
1	A	158	SER	3.0
2	B	418	ASN	3.0
1	A	159	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	148	LYS	2.9
1	A	220	LEU	2.8
2	B	321	ASP	2.8
1	A	282	LEU	2.8
2	B	318	LEU	2.7
2	B	743	THR	2.7
1	A	50	SER	2.7
1	A	223	GLU	2.7
2	B	241	MET	2.7
2	B	399	ARG	2.7
1	A	118	ILE	2.6
1	A	225	SER	2.6
2	B	323	PRO	2.6
1	A	80	GLU	2.6
1	A	81	SER	2.5
2	B	604	LEU	2.5
2	B	324	PRO	2.5
2	B	170	THR	2.4
1	A	144	GLU	2.3
1	A	92	THR	2.3
2	B	413	ARG	2.3
1	A	86	ILE	2.2
2	B	554	MET	2.2
1	A	105	SER	2.2
2	B	519	LYS	2.2
2	B	414	PHE	2.2
2	B	582	CYS	2.2
2	B	320	ASN	2.2
2	B	169	LEU	2.2
2	B	392	PHE	2.2
2	B	319	LEU	2.1
1	A	141	THR	2.1
1	A	149	LEU	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	EPE	B	801	15/15	0.86	0.21	57,80,141,153	0
4	GOL	B	802	6/6	0.86	0.26	80,90,95,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.