



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:40 pm BST

PDB ID : 4YG8
Title : CRYSTAL STRUCTURE OF THE CHS5-CHS6 EXOMER CARGO ADAPTOR COMPLEX
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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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

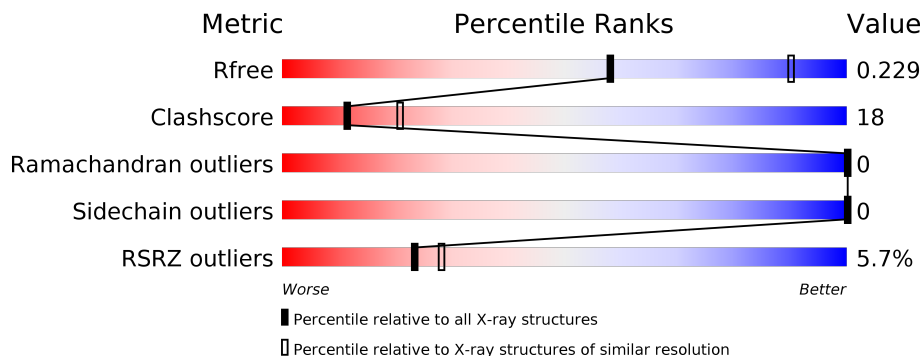
1 Overall quality at a glance

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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 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	
2	B	754	

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
			Total	C	N	O	S			
1	A	276	2082	1316	365	393	8	0	0	0

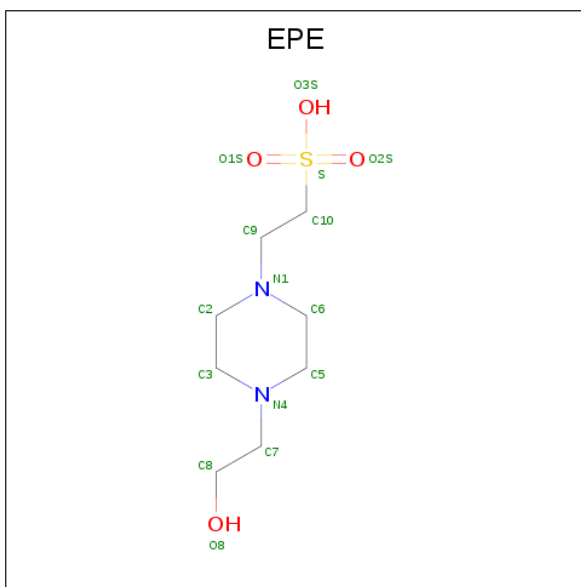
- Molecule 2 is a protein called Chitin biosynthesis protein CHS6.

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

There are 8 discrepancies between the modelled and reference sequences:

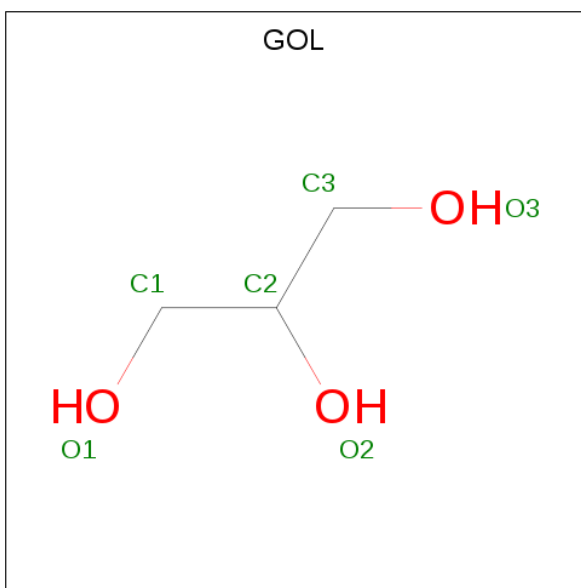
Chain	Residue	Modelled	Actual	Comment	Reference
B	747	GLY	-	expression tag	UNP P40955
B	748	THR	-	expression tag	UNP P40955
B	749	GLU	-	expression tag	UNP P40955
B	750	ASN	-	expression tag	UNP P40955
B	751	LEU	-	expression tag	UNP P40955
B	752	TYR	-	expression tag	UNP P40955
B	753	PHE	-	expression tag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

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

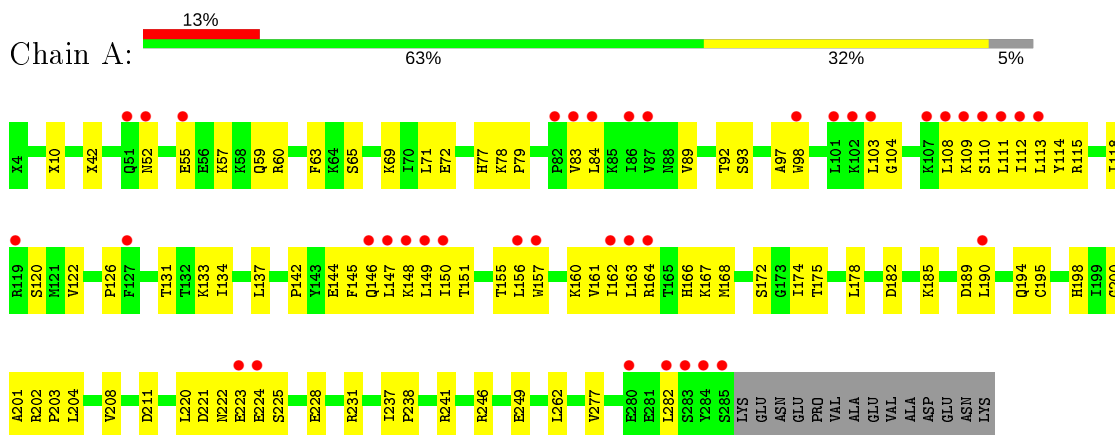
- Molecule 5 is water.

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

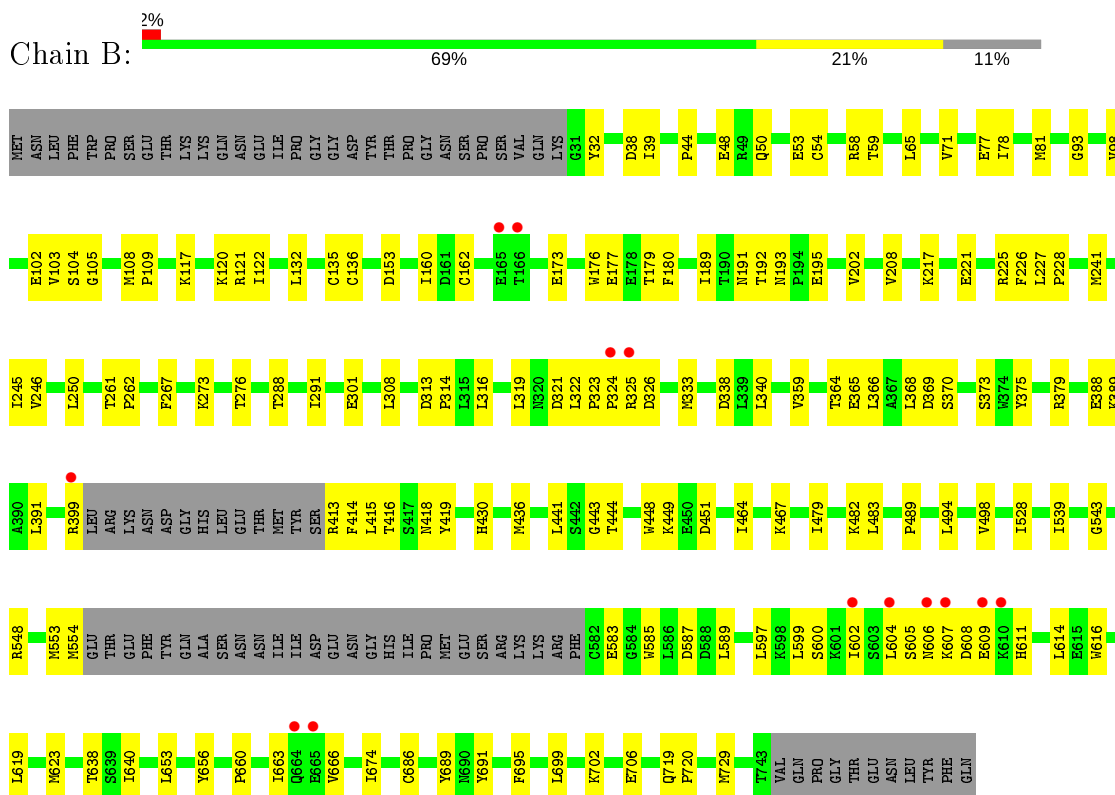
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 49.53 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.07-2.75) 90.8 (49.53-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 2.73Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.193 , 0.230 0.196 , 0.229	Depositor DCC
R_{free} test set	2856 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtrriage
Anisotropy	0.427	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.45	0/1919	0.61	0/2599
2	B	0.47	0/5555	0.59	0/7516
All	All	0.47	0/7474	0.60	0/10115

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	2082	0	1975	121	0
2	B	5446	0	5494	147	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	265	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 (265) 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: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
1:A:221:ASP:O	1:A:222:ASN:CG	1.84	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
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:HA	1:A:59:GLN:OE1	1.85	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:436:MET:HE2	2:B:436:MET:HA	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:GLU:HG3	2:B:54:CYS:N	2.04	0.72
1:A:178:LEU:HD22	1:A:204:LEU:HD21	1.72	0.72
2:B:250:LEU:HD23	2:B:250:LEU:C	2.11	0.71
1:A:175:THR:HG22	1:A:202:ARG:HB3	1.71	0.71
1:A:118:ILE:HG12	1:A:118:ILE:O	1.88	0.71
1:A:113:LEU:O	1:A:120:SER:HB2	1.89	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:HA	1:A:55:GLU:OE2	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:CG1	2:B:103:VAL:O	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:65:SER:O	1:A:69:LYS:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:MET:HG2	2:B:132:LEU:CD2	2.31	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:HA	2:B:102:GLU:OE2	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:619:LEU:HG	2:B:623:MET:HE1	1.84	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:224:GLU:O	1:A:225:SER:CB	2.49	0.59
1:A:92:THR:O	1:A:92:THR:HG22	2.01	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:365:GLU:HB3	5:B:910:HOH:O	2.03	0.58
2:B:44:PRO:HD3	2:B:689:TYR:CZ	2.39	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
1:A:133:LYS:C	1:A:134:ILE:HD13	2.24	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
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: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: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
1:A:52:ASN:ND2	1:A:55:GLU:HB2	2.20	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
1:A:161:VAL:CG1	1:A:162:ILE:N	2.69	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
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:221:ASP:O	1:A:222:ASN:CB	2.56	0.54
1:A:220:LEU:O	1:A:223:GLU:N	2.41	0.54
2:B:619:LEU:HG	2:B:623:MET:HE3	1.88	0.54
1:A:189:ASP:OD1	1:A:190:LEU:N	2.41	0.53
2:B:436:MET:CE	2:B:436:MET:HA	2.37	0.53
1:A:112:ILE:CG1	1:A:122:VAL:HG22	2.30	0.53
2:B:325:ARG:O	2:B:325:ARG:HG2	2.08	0.53
1:A:79:PRO:HB2	1:A:103:LEU:HD23	1.91	0.52
2:B:313:ASP:HB2	2:B:314:PRO:HD3	1.92	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
2:B:441:LEU:O	2:B:444:THR:OG1	2.23	0.50
1:A:147:LEU:O	1:A:157:TRP:CB	2.59	0.50
2:B:58:ARG:HD2	2:B:78:ILE:HD11	1.93	0.50
1:A:114:TYR:CE2	1:A:118:ILE:HB	2.46	0.50
1:A:108:LEU:HD11	1:A:149:LEU:HD12	1.93	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:167:LYS:HG2	1:A:168:MET:N	2.27	0.49
2:B:250:LEU:O	2:B:250:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:224:GLU:O	1:A:225:SER:OG	2.30	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:415:LEU:O	2:B:415:LEU:HG	2.14	0.48
2:B:191:ASN:O	3:B:801:EPE:H22	2.12	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:N	1:A:134:ILE:HD13	2.28	0.47
2:B:430:HIS:N	2:B:430:HIS:CD2	2.81	0.47
1:A:71:LEU:O	1:A:72:GLU:C	2.50	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
2:B:464:ILE:O	2:B:464:ILE:HG13	2.14	0.47
1:A:175:THR:HG22	1:A:202:ARG:CB	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
1:A:60:ARG:HG2	2:B:316:LEU:CD2	2.44	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:291:ILE:HD13	2:B:308:LEU:HD23	1.97	0.46
1:A:57:LYS:HA	1:A:60:ARG:NH2	2.30	0.46
1:A:92:THR:CG2	1:A:92:THR:O	2.64	0.46
2:B:250:LEU:CD2	2:B:250:LEU:C	2.83	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:H	2:B:430:HIS:CD2	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:208:VAL:HB	1:A:231:ARG:HD2	2.00	0.44
1:A:190:LEU:HD23	1:A:277:VAL:HG11	2.00	0.44
2:B:388:GLU:N	2:B:388:GLU:OE1	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:HA	2:B:619:LEU:HD12	1.71	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:539:ILE:HG13	2:B:543:GLY:HA3	1.99	0.43
2:B:173:GLU:OE1	2:B:173:GLU:HA	2.19	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
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:104:SER:HA	2:B:180:PHE:HB2	2.02	0.42
2:B:98:VAL:HA	2:B:202:VAL:O	2.20	0.42
2:B:323:PRO:N	2:B:324:PRO:HD2	2.30	0.42
2:B:326:ASP:N	2:B:326:ASP:OD1	2.52	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:LEU:HD12	2:B:415:LEU:C	2.40	0.41
2:B:653:LEU:HB3	2:B:699:LEU:HD11	2.01	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:174:ILE:O	1:A:201:ALA:HB1	2.21	0.41
1:A:79:PRO:CB	1:A:103:LEU:HD22	2.44	0.41
2:B:78:ILE:HG12	2:B:135:CYS:HB2	2.03	0.41
1:A:118:ILE:O	1:A:120:SER:O	2.39	0.41
2:B:448:TRP:CZ2	2:B:464:ILE:HB	2.56	0.41
2:B:53:GLU:HG3	2:B:54:CYS:H	1.83	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:HA	2:B:674:ILE:HD13	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: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 [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	234/290 (81%)	226 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [i](#)

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%)	218 (100%)	0	100	100
2	B	616/690 (89%)	616 (100%)	0	100	100
All	All	834/920 (91%)	834 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

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
3	EPE	B	801	-	15,15,15	0.89	1 (6%)	18,20,20	1.34	2 (11%)
4	GOL	B	802	-	5,5,5	0.31	0	5,5,5	0.68	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	EPE	B	801	-	-	4/9/19/19	0/1/1/1
4	GOL	B	802	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	EPE	C10-S	3.01	1.81	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	EPE	O3S-S-C10	2.57	109.92	105.77
3	B	801	EPE	C6-N1-C2	2.16	113.70	108.83

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

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Mol	Chain	Res	Type	Atoms
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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	0.67	39 (16%) 1 1	35, 83, 150, 175	0
2	B	673/754 (89%)	-0.07	13 (1%) 66 75	24, 49, 109, 182	0
All	All	909/1044 (87%)	0.12	52 (5%) 23 28	24, 55, 129, 182	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	LEU	5.4
2	B	604	LEU	5.1
2	B	609	GLU	5.0
1	A	163	LEU	4.9
1	A	284	TYR	4.5
1	A	149	LEU	4.4
2	B	610	LYS	4.4
1	A	146	GLN	4.4
1	A	101	LEU	4.4
1	A	282	LEU	4.4
1	A	119	ARG	4.4
1	A	127	PHE	4.3
2	B	325	ARG	4.1
1	A	164	ARG	4.0
2	B	607	LYS	4.0
1	A	147	LEU	3.9
1	A	103	LEU	3.8
2	B	606	ASN	3.8
1	A	109	LYS	3.7
1	A	112	ILE	3.6
1	A	283	SER	3.6
1	A	51	GLN	3.6
1	A	110	SER	3.4
1	A	156	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	148	LYS	3.4
1	A	98	TRP	3.4
1	A	280	GLU	3.3
2	B	665	GLU	3.3
1	A	86	ILE	3.2
1	A	111	LEU	3.2
1	A	162	ILE	3.1
1	A	52	ASN	3.1
1	A	113	LEU	3.1
2	B	399	ARG	3.0
2	B	664	GLN	2.9
1	A	107	LYS	2.8
1	A	150	ILE	2.7
1	A	84	LEU	2.7
1	A	83	VAL	2.7
2	B	165	GLU	2.4
1	A	224	GLU	2.4
2	B	324	PRO	2.3
1	A	285	SER	2.3
1	A	87	VAL	2.3
1	A	102	LYS	2.3
1	A	55	GLU	2.2
1	A	82	PRO	2.2
2	B	166	THR	2.1
1	A	190	LEU	2.1
2	B	602	ILE	2.1
1	A	157	TRP	2.1
1	A	223	GLU	2.1

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. 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(Å ²)	Q<0.9
4	GOL	B	802	6/6	0.81	0.30	80,90,95,98	0
3	EPE	B	801	15/15	0.92	0.30	57,80,141,153	0

6.5 Other polymers [i](#)

There are no such residues in this entry.