Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 02:05 am BST

PDB ID	:	6HUE
Title	:	ParkinS65N
Authors	:	McWilliams, T.G.; Barini, E.; Pohjolan-Pirhonen, R.; Brooks, S.P.; Singh, F.; Burel, S.; Balk, K.; Kumar, A.; Montava-Garriga, L.; Prescott, A.R.; Hassoun, S.M.; Mouton-Liger, F.; Ball, G.; Hills, R.; Knebel, A.; Ulusoy, A.; Di Monte, D.A.; Tamjar, J.; Antico, O.; Fears, K.; Smith, L.; Brambilla, R.; Palin, E.; Valori, M.; Eerola-Rautio, J.; Tienari, P.; Corti, O.; Dunnett, S.B.; Ganley, I.G.; Suomalainen, A.; Muqit, M.M.K.
Deposited on	:	2018-10-07
Resolution	:	2.85 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

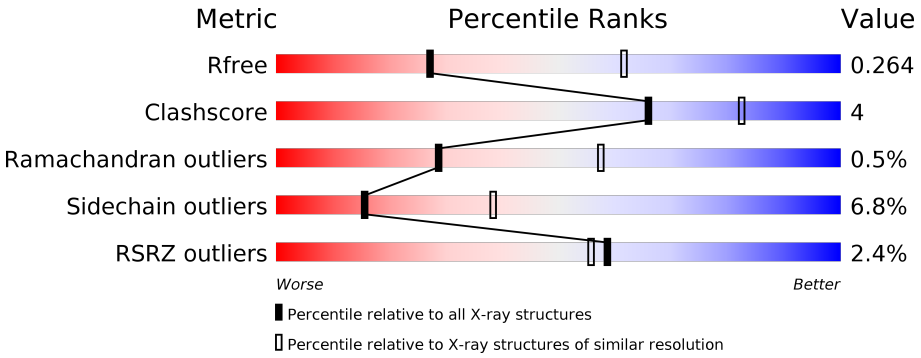
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 <=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	405	2% 80% 13% • 7%
1	B	405	2% 80% 13% 6%

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
5	CL	A	512	-	-	X	-
5	CL	B	512	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6333 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 E3 ubiquitin-protein ligase parkin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	12	0
			3053	1902	556	553	42			
1	B	382	Total	C	N	O	S	0	11	0
			3071	1912	560	557	42			

There are 122 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	ASN	SER	engineered mutation	UNP O60260
A	?	-	GLY	deletion	UNP O60260
A	?	-	GLY	deletion	UNP O60260
A	?	-	ASP	deletion	UNP O60260
A	?	-	ASP	deletion	UNP O60260
A	?	-	PRO	deletion	UNP O60260
A	?	-	ARG	deletion	UNP O60260
A	?	-	ASN	deletion	UNP O60260
A	?	-	ALA	deletion	UNP O60260
A	?	-	ALA	deletion	UNP O60260
A	?	-	GLY	deletion	UNP O60260
A	?	-	GLY	deletion	UNP O60260
A	?	-	CYS	deletion	UNP O60260
A	?	-	GLU	deletion	UNP O60260
A	?	-	ARG	deletion	UNP O60260
A	?	-	GLU	deletion	UNP O60260
A	?	-	PRO	deletion	UNP O60260
A	?	-	GLN	deletion	UNP O60260
A	?	-	SER	deletion	UNP O60260
A	?	-	LEU	deletion	UNP O60260
A	?	-	THR	deletion	UNP O60260
A	?	-	ARG	deletion	UNP O60260
A	?	-	VAL	deletion	UNP O60260
A	?	-	ASP	deletion	UNP O60260
A	?	-	LEU	deletion	UNP O60260

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP O60260
A	?	-	SER	deletion	UNP O60260
A	?	-	SER	deletion	UNP O60260
A	?	-	VAL	deletion	UNP O60260
A	?	-	LEU	deletion	UNP O60260
A	?	-	PRO	deletion	UNP O60260
A	?	-	GLY	deletion	UNP O60260
A	?	-	ASP	deletion	UNP O60260
A	?	-	SER	deletion	UNP O60260
A	?	-	VAL	deletion	UNP O60260
A	?	-	GLY	deletion	UNP O60260
A	?	-	LEU	deletion	UNP O60260
A	?	-	ALA	deletion	UNP O60260
A	?	-	VAL	deletion	UNP O60260
A	?	-	ILE	deletion	UNP O60260
A	?	-	LEU	deletion	UNP O60260
A	?	-	HIS	deletion	UNP O60260
A	?	-	THR	deletion	UNP O60260
A	?	-	ASP	deletion	UNP O60260
A	?	-	SER	deletion	UNP O60260
A	?	-	ARG	deletion	UNP O60260
A	?	-	LYS	deletion	UNP O60260
A	?	-	ASP	deletion	UNP O60260
A	?	-	SER	deletion	UNP O60260
A	?	-	PRO	deletion	UNP O60260
A	?	-	PRO	deletion	UNP O60260
A	?	-	ALA	deletion	UNP O60260
A	?	-	GLY	deletion	UNP O60260
A	?	-	SER	deletion	UNP O60260
A	?	-	PRO	deletion	UNP O60260
A	?	-	ALA	deletion	UNP O60260
A	?	-	GLY	deletion	UNP O60260
A	?	-	ARG	deletion	UNP O60260
A	?	-	SER	deletion	UNP O60260
A	?	-	ILE	deletion	UNP O60260
A	?	-	TYR	deletion	UNP O60260
B	65	ASN	SER	engineered mutation	UNP O60260
B	?	-	GLY	deletion	UNP O60260
B	?	-	GLY	deletion	UNP O60260
B	?	-	ASP	deletion	UNP O60260
B	?	-	ASP	deletion	UNP O60260
B	?	-	PRO	deletion	UNP O60260

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ARG	deletion	UNP O60260
B	?	-	ASN	deletion	UNP O60260
B	?	-	ALA	deletion	UNP O60260
B	?	-	ALA	deletion	UNP O60260
B	?	-	GLY	deletion	UNP O60260
B	?	-	GLY	deletion	UNP O60260
B	?	-	CYS	deletion	UNP O60260
B	?	-	GLU	deletion	UNP O60260
B	?	-	ARG	deletion	UNP O60260
B	?	-	GLU	deletion	UNP O60260
B	?	-	PRO	deletion	UNP O60260
B	?	-	GLN	deletion	UNP O60260
B	?	-	SER	deletion	UNP O60260
B	?	-	LEU	deletion	UNP O60260
B	?	-	THR	deletion	UNP O60260
B	?	-	ARG	deletion	UNP O60260
B	?	-	VAL	deletion	UNP O60260
B	?	-	ASP	deletion	UNP O60260
B	?	-	LEU	deletion	UNP O60260
B	?	-	SER	deletion	UNP O60260
B	?	-	SER	deletion	UNP O60260
B	?	-	SER	deletion	UNP O60260
B	?	-	VAL	deletion	UNP O60260
B	?	-	LEU	deletion	UNP O60260
B	?	-	PRO	deletion	UNP O60260
B	?	-	GLY	deletion	UNP O60260
B	?	-	ASP	deletion	UNP O60260
B	?	-	SER	deletion	UNP O60260
B	?	-	VAL	deletion	UNP O60260
B	?	-	GLY	deletion	UNP O60260
B	?	-	LEU	deletion	UNP O60260
B	?	-	ALA	deletion	UNP O60260
B	?	-	VAL	deletion	UNP O60260
B	?	-	ILE	deletion	UNP O60260
B	?	-	LEU	deletion	UNP O60260
B	?	-	HIS	deletion	UNP O60260
B	?	-	THR	deletion	UNP O60260
B	?	-	ASP	deletion	UNP O60260
B	?	-	SER	deletion	UNP O60260
B	?	-	ARG	deletion	UNP O60260
B	?	-	LYS	deletion	UNP O60260
B	?	-	ASP	deletion	UNP O60260

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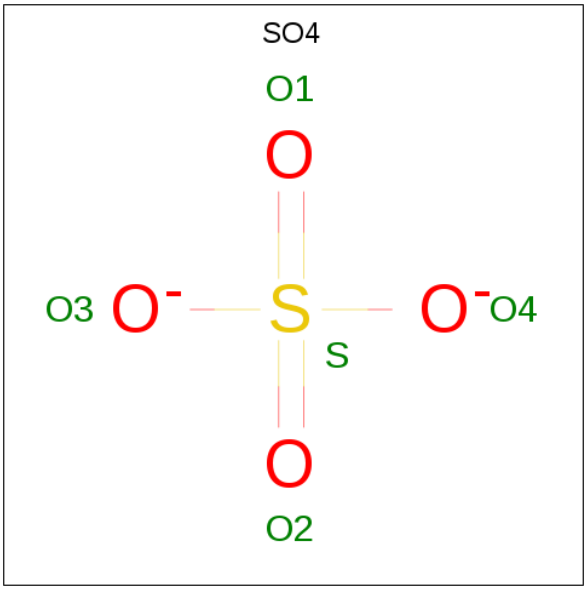
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP O60260
B	?	-	PRO	deletion	UNP O60260
B	?	-	PRO	deletion	UNP O60260
B	?	-	ALA	deletion	UNP O60260
B	?	-	GLY	deletion	UNP O60260
B	?	-	SER	deletion	UNP O60260
B	?	-	PRO	deletion	UNP O60260
B	?	-	ALA	deletion	UNP O60260
B	?	-	GLY	deletion	UNP O60260
B	?	-	ARG	deletion	UNP O60260
B	?	-	SER	deletion	UNP O60260
B	?	-	ILE	deletion	UNP O60260
B	?	-	TYR	deletion	UNP O60260

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

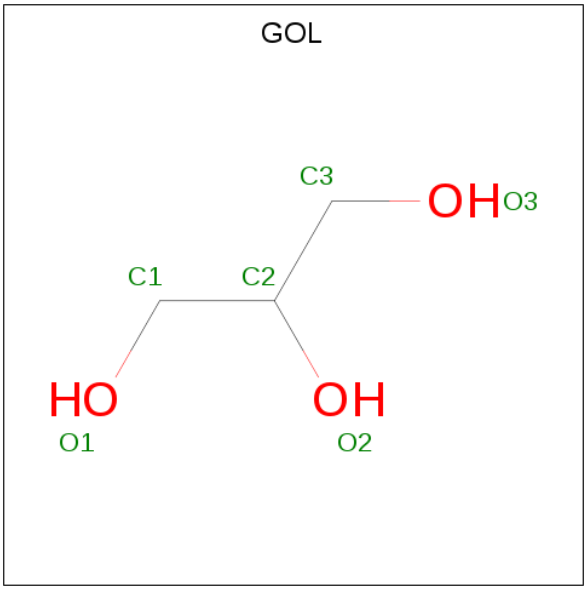
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	8	Total Zn 8 8	0	0
2	A	8	Total Zn 8 8	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is water.

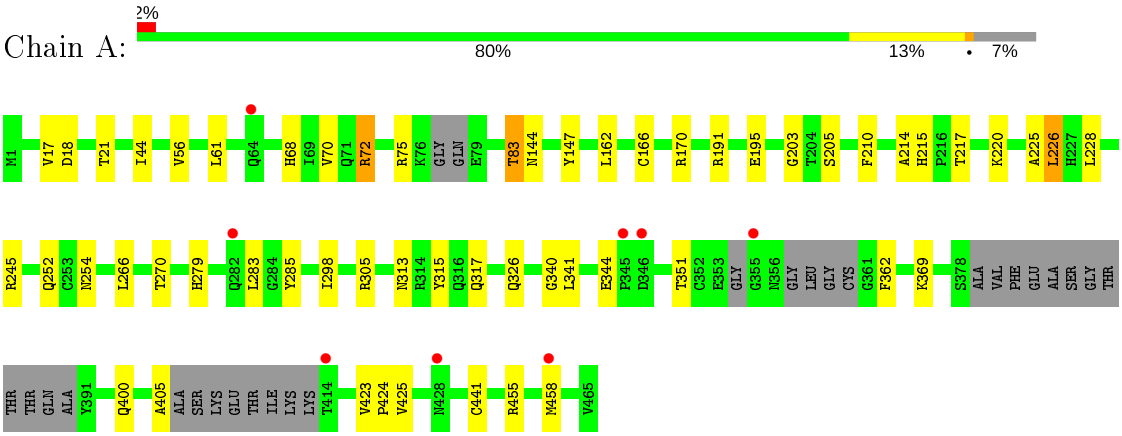
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	87	Total O 87 87	0	0
6	B	70	Total O 70 70	0	0

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.

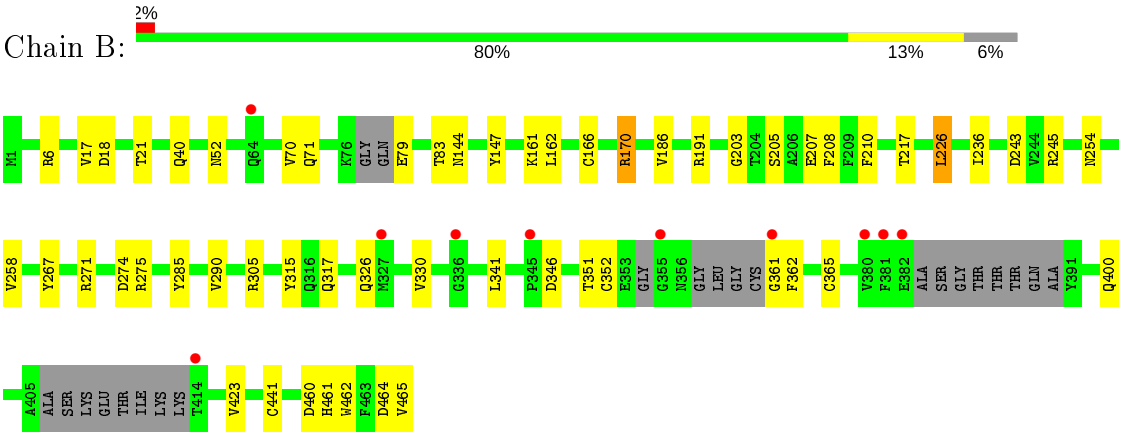
- Molecule 1: E3 ubiquitin-protein ligase parkin

Chain A:



- Molecule 1: E3 ubiquitin-protein ligase parkin

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.43Å 66.87Å 206.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.98 – 2.85 47.98 – 2.85	Depositor EDS
% Data completeness (in resolution range)	95.0 (47.98-2.85) 93.4 (47.98-2.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.223 , 0.255 0.229 , 0.264	Depositor DCC
R_{free} test set	1095 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.418 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6333	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, ZN, SO4, CL

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	0.55	0/3154	0.77	0/4265
1	B	0.55	0/3169	0.79	1/4286 (0.0%)
All	All	0.55	0/6323	0.78	1/8551 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	275	ARG	NE-CZ-NH2	5.47	123.04	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3053	0	2922	25	0
1	B	3071	0	2931	23	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	12	0	16	1	0
4	B	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	2	0
5	B	1	0	0	2	0
6	A	87	0	0	5	0
6	B	70	0	0	4	0
All	All	6333	0	5885	48	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 4.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:VAL:HG12	1:A:21:THR:HG21	1.73	0.71
1:B:83:THR:HG1	1:B:144:ASN:N	1.90	0.70
1:B:236:ILE:HG21	1:B:258:VAL:HG21	1.74	0.69
1:B:147:TYR:N	5:B:512:CL:CL	2.67	0.64
1:A:83:THR:O	1:A:144:ASN:N	2.31	0.63
1:B:243[A]:ASP:OD2	1:B:245[A]:ARG:HD3	1.98	0.63
1:A:162:LEU:HD13	1:A:210:PHE:CE1	2.41	0.55
1:A:340:GLY:C	1:A:341:LEU:HD12	2.27	0.55
1:B:267:TYR:CE1	1:B:290:VAL:HG23	2.42	0.54
1:B:285:TYR:O	1:B:315:TYR:OH	2.12	0.54
1:A:83:THR:HG21	6:A:671:HOH:O	2.07	0.54
1:B:17:VAL:HG12	1:B:21:THR:HG21	1.91	0.51
1:B:83:THR:OG1	1:B:144:ASN:N	2.44	0.50
1:A:254[A]:ASN:HB3	6:A:614:HOH:O	2.12	0.48
1:B:423:VAL:HB	6:B:639:HOH:O	2.14	0.48
1:A:162:LEU:HD13	1:A:210:PHE:CZ	2.49	0.47
1:B:6:ARG:NH1	1:B:274:ASP:OD1	2.47	0.47
1:A:266:LEU:O	1:A:270:THR:HG23	2.15	0.47
1:B:226:LEU:O	5:B:512:CL:CL	2.70	0.46
1:B:83:THR:OG1	1:B:460:ASP:OD2	2.33	0.46
1:A:44:ILE:HB	1:A:68:HIS:HB2	1.98	0.46
1:B:162:LEU:HD13	1:B:210:PHE:CE2	2.51	0.45
1:A:405:ALA:C	6:A:665:HOH:O	2.54	0.45
1:B:40:GLN:NE2	1:B:71:GLN:HE21	2.14	0.45
1:A:279:HIS:HB2	1:A:285:TYR:CE1	2.53	0.45
1:A:285:TYR:O	1:A:315:TYR:OH	2.24	0.45
1:A:228:LEU:HD11	1:A:298:ILE:HG23	1.99	0.44
1:A:369:LYS:HE2	6:A:650:HOH:O	2.17	0.44
1:A:44:ILE:HG21	1:A:270:THR:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:GLY:N	6:B:602:HOH:O	2.51	0.43
1:A:75:ARG:O	1:A:245[B]:ARG:NH2	2.52	0.43
1:A:56:VAL:HG13	1:A:61:LEU:HB2	1.99	0.43
1:A:72:ARG:HG2	6:A:639:HOH:O	2.18	0.43
1:B:83:THR:O	1:B:144:ASN:N	2.52	0.43
1:B:161:LYS:NZ	6:B:603:HOH:O	2.51	0.43
1:B:465:VAL:O	1:B:465:VAL:HG23	2.19	0.42
1:A:313:ASN:O	1:A:317:GLN:HG2	2.19	0.42
1:A:252:GLN:HE22	4:A:511:GOL:H32	1.85	0.42
1:B:254[B]:ASN:HB2	6:B:644:HOH:O	2.19	0.42
1:A:210:PHE:CD2	1:A:225:ALA:HB2	2.55	0.41
1:B:170:ARG:HD2	1:B:207:GLU:OE1	2.20	0.41
1:B:186:VAL:HG12	1:B:208:PHE:CG	2.55	0.41
1:A:214:ALA:HB3	1:A:215:HIS:HD2	1.85	0.41
1:B:162:LEU:HD13	1:B:210:PHE:CZ	2.56	0.41
1:B:461:HIS:O	1:B:462:TRP:C	2.59	0.41
1:A:147:TYR:N	5:A:512:CL:CL	2.78	0.41
1:A:423:VAL:HG13	1:A:424:PRO:HD2	2.03	0.40
1:A:226:LEU:O	5:A:512:CL:CL	2.77	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	376/405 (93%)	349 (93%)	25 (7%)	2 (0%)	29 57
1	B	379/405 (94%)	352 (93%)	25 (7%)	2 (0%)	29 57
All	All	755/810 (93%)	701 (93%)	50 (7%)	4 (0%)	29 57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	GLY
1	A	283	LEU
1	B	203	GLY
1	B	52	ASN

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	344/353 (98%)	321 (93%)	23 (7%)	16	39
1	B	344/353 (98%)	321 (93%)	23 (7%)	16	39
All	All	688/706 (98%)	642 (93%)	46 (7%)	16	39

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	70	VAL
1	A	72	ARG
1	A	83	THR
1	A	166	CYS
1	A	170	ARG
1	A	191	ARG
1	A	195	GLU
1	A	205	SER
1	A	217	THR
1	A	220	LYS
1	A	226	LEU
1	A	305	ARG
1	A	326	GLN
1	A	344	GLU
1	A	351	THR
1	A	362	PHE
1	A	400	GLN
1	A	425	VAL
1	A	441	CYS

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Mol	Chain	Res	Type
1	A	455	ARG
1	A	458[A]	MET
1	A	458[B]	MET
1	B	18	ASP
1	B	70	VAL
1	B	79	GLU
1	B	166	CYS
1	B	170	ARG
1	B	191	ARG
1	B	205	SER
1	B	217	THR
1	B	226	LEU
1	B	271	ARG
1	B	305	ARG
1	B	317	GLN
1	B	326	GLN
1	B	330	VAL
1	B	341	LEU
1	B	346	ASP
1	B	351	THR
1	B	352	CYS
1	B	362	PHE
1	B	365	CYS
1	B	400	GLN
1	B	441	CYS
1	B	464	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	144	ASN
1	A	252	GLN
1	A	295	ASN
1	A	317	GLN
1	A	326	GLN
1	A	400	GLN
1	B	34	GLN
1	B	40	GLN
1	B	144	ASN
1	B	326	GLN
1	B	400	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

Of 24 ligands modelled in this entry, 18 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	B	510	-	5,5,5	0.41	0	5,5,5	0.29	0
3	SO4	A	509	-	4,4,4	0.34	0	6,6,6	0.72	0
4	GOL	A	511	-	5,5,5	0.29	0	5,5,5	0.46	0
4	GOL	B	511	-	5,5,5	0.27	0	5,5,5	0.28	0
3	SO4	B	509	-	4,4,4	0.33	0	6,6,6	0.54	0
4	GOL	A	510	-	5,5,5	0.29	0	5,5,5	0.32	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
4	GOL	B	511	-	-	2/4/4/4	-
4	GOL	A	511	-	-	0/4/4/4	-
4	GOL	B	510	-	-	0/4/4/4	-
4	GOL	A	510	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	511	GOL	O1-C1-C2-C3
4	B	511	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	511	GOL	1	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	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	83:THR	C	144:ASN	N	2.92
1	B	83:THR	C	144:ASN	N	2.81

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, 95^{th} 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	378/405 (93%)	-0.01	8 (2%)	63	60	39, 62, 96, 139	0
1	B	382/405 (94%)	0.05	10 (2%)	56	52	39, 62, 103, 135	0
All	All	760/810 (93%)	0.02	18 (2%)	59	56	39, 62, 99, 139	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	GLU	5.1
1	B	380	VAL	3.5
1	A	414	THR	3.5
1	A	345	PRO	3.5
1	A	346	ASP	3.4
1	B	355	GLY	2.9
1	B	345	PRO	2.8
1	A	428	ASN	2.7
1	A	282	GLN	2.7
1	B	336	GLY	2.6
1	B	64	GLN	2.5
1	B	381	PHE	2.5
1	A	355	GLY	2.3
1	A	64	GLN	2.2
1	B	361	GLY	2.1
1	B	414	THR	2.1
1	B	327	MET	2.0
1	A	458[A]	MET	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 (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, 95^{th} 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
5	CL	B	512	1/1	0.83	0.43	101,101,101,101	0
4	GOL	B	510	6/6	0.92	0.18	61,68,69,71	0
5	CL	A	512	1/1	0.93	0.38	84,84,84,84	0
4	GOL	A	510	6/6	0.94	0.14	55,56,56,61	0
4	GOL	A	511	6/6	0.94	0.21	53,54,57,58	0
4	GOL	B	511	6/6	0.95	0.16	47,47,48,48	0
3	SO4	A	509	5/5	0.97	0.16	47,51,55,58	0
2	ZN	A	505	1/1	0.97	0.11	87,87,87,87	0
2	ZN	B	506	1/1	0.98	0.09	76,76,76,76	0
2	ZN	A	502	1/1	0.99	0.13	52,52,52,52	0
2	ZN	A	504	1/1	0.99	0.15	61,61,61,61	0
2	ZN	B	508	1/1	0.99	0.13	55,55,55,55	0
2	ZN	A	501	1/1	0.99	0.15	42,42,42,42	0
2	ZN	B	507	1/1	0.99	0.12	72,72,72,72	0
2	ZN	A	507	1/1	0.99	0.14	73,73,73,73	0
2	ZN	B	505	1/1	0.99	0.10	90,90,90,90	0
2	ZN	B	504	1/1	0.99	0.14	59,59,59,59	0
3	SO4	B	509	5/5	0.99	0.14	49,49,53,58	0
2	ZN	B	501	1/1	0.99	0.13	44,44,44,44	0
2	ZN	A	506	1/1	0.99	0.09	79,79,79,79	0
2	ZN	A	503	1/1	1.00	0.15	40,40,40,40	0
2	ZN	A	508	1/1	1.00	0.12	53,53,53,53	0
2	ZN	B	503	1/1	1.00	0.14	48,48,48,48	0
2	ZN	B	502	1/1	1.00	0.12	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.