



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 02:51 pm BST

PDB ID : 2XRE
Title : Detection of cobalt in previously unassigned human SENP1 structure
Authors : Rimsa, V.; Eadsforth, T.; Hay, R.T.; Hunter, W.N.
Deposited on : 2010-09-14
Resolution : 2.45 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

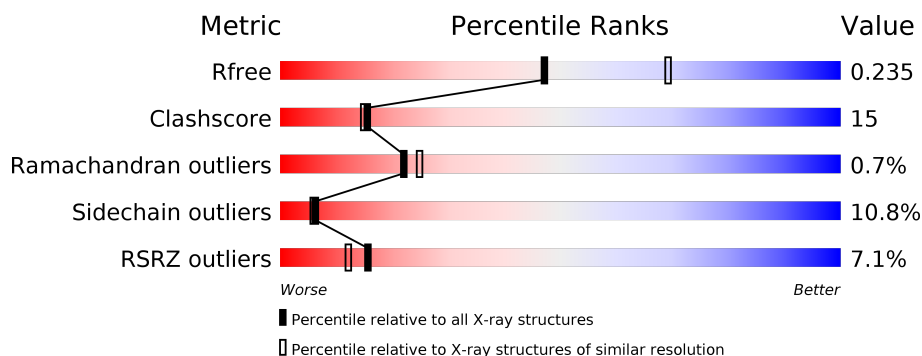
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	230	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>22%</div> <div>5% •</div> </div> </div>
1	B	230	<div> <div>10%</div> <div> <div></div> <div>60%</div> <div>31%</div> <div>5% ••</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3952 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 SENTRIN-SPECIFIC PROTEASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	4	0
			1911	1226	330	342	13			
1	B	226	Total	C	N	O	S	0	9	0
			1919	1232	333	340	14			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Co	0	0
			1	1		

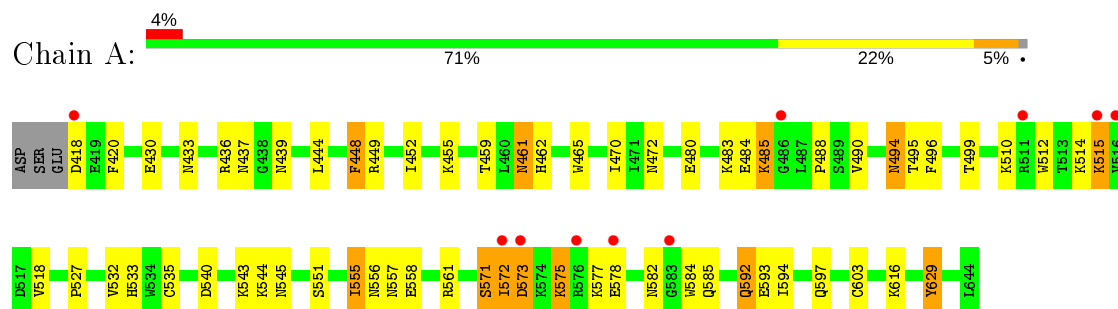
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	26	Total	O	0	0
			26	26		

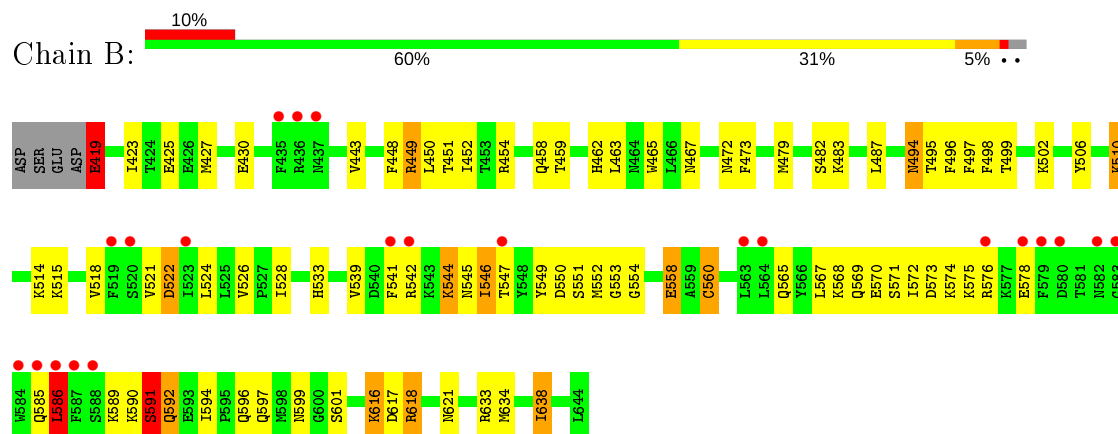
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: SENTRIN-SPECIFIC PROTEASE 1



• Molecule 1: SENTRIN-SPECIFIC PROTEASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.98Å 71.98Å 200.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.60 – 2.45 45.60 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.60-2.45) 100.0 (45.60-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.237 , 0.317 0.239 , 0.235	Depositor DCC
R_{free} test set	1141 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3952	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% 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, CO

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	0.78	0/1956	0.78	0/2634
1	B	0.97	9/1976 (0.5%)	1.20	22/2658 (0.8%)
All	All	0.88	9/3932 (0.2%)	1.01	22/5292 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	590	LYS	C-O	-10.61	1.03	1.23
1	B	576	ARG	C-O	-9.99	1.04	1.23
1	B	592	GLN	C-O	-9.63	1.05	1.23
1	B	591	SER	CA-CB	-8.47	1.40	1.52
1	B	483	LYS	CG-CD	8.46	1.81	1.52
1	B	591	SER	CB-OG	8.27	1.52	1.42
1	B	482	SER	N-CA	-7.58	1.31	1.46
1	B	591	SER	CA-C	-5.23	1.39	1.52
1	B	560	CYS	CB-SG	5.22	1.91	1.82

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	483	LYS	CG-CD-CE	-18.33	56.91	111.90
1	B	419	GLU	CA-C-O	-16.61	85.21	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	592	GLN	O-C-N	16.50	149.10	122.70
1	B	419	GLU	CA-C-N	14.33	148.72	117.20
1	B	592	GLN	CB-CA-C	14.02	138.45	110.40
1	B	591	SER	O-C-N	-12.24	103.12	122.70
1	B	592	GLN	CA-C-N	-11.92	90.98	117.20
1	B	592	GLN	C-N-CA	-10.62	95.14	121.70
1	B	483	LYS	CB-CG-CD	-9.45	87.03	111.60
1	B	591	SER	CA-CB-OG	9.26	136.21	111.20
1	B	482	SER	N-CA-CB	7.13	121.19	110.50
1	B	590	LYS	O-C-N	-7.06	111.41	122.70
1	B	638[A]	ILE	CA-C-N	6.54	131.59	117.20
1	B	638[B]	ILE	CA-C-N	6.54	131.59	117.20
1	B	591	SER	CB-CA-C	6.32	122.10	110.10
1	B	638[A]	ILE	CA-C-O	-5.94	107.63	120.10
1	B	638[B]	ILE	CA-C-O	-5.94	107.63	120.10
1	B	575	LYS	N-CA-C	5.89	126.92	111.00
1	B	578	GLU	N-CA-C	-5.54	96.03	111.00
1	B	419	GLU	C-N-CA	-5.54	107.86	121.70
1	B	586	LEU	CA-CB-CG	5.34	127.58	115.30
1	B	575	LYS	C-N-CA	5.05	134.33	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	574	LYS	Mainchain
1	B	591	SER	Mainchain

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	1911	0	1868	49	2
1	B	1919	0	1875	71	1
2	A	24	0	32	1	0
2	B	36	0	48	4	0
3	B	1	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	35	0	0	0	0
4	B	26	0	0	2	0
All	All	3952	0	3823	114	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (114) 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:419:GLU:O	1:B:419:GLU:CG	1.64	1.22
1:B:449[B]:ARG:HH11	1:B:449[B]:ARG:CG	1.63	1.12
1:A:465[A]:TRP:CZ3	1:B:558:GLU:HG3	1.87	1.08
1:B:449[B]:ARG:NH1	1:B:449[B]:ARG:HG2	1.60	1.07
1:A:465[A]:TRP:CH2	1:B:558:GLU:HG3	1.89	1.05
1:A:461:ASN:ND2	1:A:462:HIS:H	1.56	1.04
1:B:449[B]:ARG:HH11	1:B:449[B]:ARG:HG2	0.84	1.01
1:B:546:ILE:HD11	1:B:560:CYS:HB3	1.41	0.98
1:A:461:ASN:HD22	1:A:462:HIS:N	1.65	0.94
1:A:461:ASN:HD22	1:A:462:HIS:H	0.94	0.92
1:A:514:LYS:O	1:A:515:LYS:HG3	1.71	0.91
1:B:510:LYS:O	1:B:510:LYS:HD2	1.75	0.86
1:B:419:GLU:HG2	1:B:419:GLU:O	1.05	0.86
1:A:465[A]:TRP:CZ3	1:B:558:GLU:CG	2.64	0.79
1:B:618[B]:ARG:CZ	2:B:1646:GOL:H11	2.12	0.79
1:A:465[A]:TRP:HZ3	1:B:558:GLU:CG	1.96	0.78
1:B:571:SER:C	1:B:571:SER:N	2.40	0.75
1:B:494:ASN:HD21	1:B:496:PHE:HD1	1.35	0.74
1:A:465[A]:TRP:HZ3	1:B:558:GLU:HG3	1.47	0.72
1:A:461:ASN:ND2	1:A:462:HIS:N	2.30	0.72
1:A:465[A]:TRP:HH2	1:B:558:GLU:HG3	1.51	0.72
1:B:565:GLN:O	1:B:569:GLN:HG3	1.89	0.71
1:A:572:ILE:HG22	1:A:573:ASP:N	2.06	0.70
1:B:465[B]:TRP:CD1	1:B:601:SER:HA	2.27	0.70
1:B:510:LYS:O	1:B:510:LYS:CD	2.40	0.70
1:A:448:PHE:O	1:A:449:ARG:HB2	1.91	0.70
1:A:532:VAL:HG22	4:B:2014:HOH:O	1.92	0.69
1:A:555:ILE:HG13	1:A:556:ASN:N	2.06	0.69
1:B:618[B]:ARG:NH1	2:B:1646:GOL:H11	2.07	0.68
1:A:551:SER:O	1:A:597:GLN:HG2	1.94	0.68
1:A:472:ASN:OD1	1:A:495:THR:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:SER:OG	1:B:597:GLN:NE2	2.29	0.66
1:B:423:ILE:HG23	1:B:427:MET:HB2	1.77	0.64
1:B:510:LYS:HD3	1:B:570:GLU:OE2	1.98	0.64
1:A:465[A]:TRP:HZ3	1:B:558:GLU:CD	2.00	0.63
1:A:452:ILE:HD12	1:A:470:ILE:HD13	1.80	0.63
1:A:544:LYS:O	1:A:584:TRP:HA	1.98	0.63
1:B:539:VAL:HG22	1:B:546:ILE:HG22	1.82	0.62
1:B:634:MET:O	1:B:638[B]:ILE:HG22	1.99	0.62
1:A:551:SER:OG	1:A:597:GLN:NE2	2.31	0.62
1:B:506:TYR:CD2	2:B:1647:GOL:H32	2.36	0.61
1:B:616:LYS:O	1:B:617:ASP:HB2	2.02	0.60
1:A:592:GLN:OE1	1:A:593:GLU:HG3	2.02	0.59
1:B:462[B]:HIS:CD2	1:B:463:LEU:HG	2.37	0.59
1:B:454:ARG:O	1:B:458:GLN:HG2	2.04	0.57
1:A:557:ASN:OD1	1:A:561:ARG:NH1	2.36	0.57
1:B:533:HIS:CE1	1:B:552:MET:HB2	2.40	0.57
1:B:546:ILE:C	1:B:546:ILE:HD12	2.25	0.57
1:A:551:SER:HG	1:A:597:GLN:HE21	1.53	0.56
1:A:480:GLU:HG2	2:A:1645:GOL:H12	1.87	0.56
1:A:512:TRP:N	1:A:512:TRP:CD1	2.73	0.56
1:B:465[B]:TRP:NE1	1:B:601:SER:HA	2.20	0.56
1:A:465[B]:TRP:CZ3	1:A:603:CYS:SG	2.99	0.56
1:B:423:ILE:HG23	1:B:427:MET:CB	2.37	0.55
1:B:425[A]:GLU:H	1:B:425[A]:GLU:CD	2.11	0.55
1:A:495:THR:HA	1:A:527:PRO:HG2	1.89	0.53
1:B:568:LYS:O	1:B:572:ILE:HD12	2.09	0.53
1:B:565:GLN:C	1:B:569:GLN:HE21	2.13	0.52
1:A:510:LYS:NZ	1:A:573:ASP:OD2	2.31	0.51
1:A:571:SER:O	1:A:575:LYS:HB2	2.11	0.50
1:B:545:ASN:HB3	1:B:585:GLN:OE1	2.12	0.49
1:A:461:ASN:O	1:A:462:HIS:C	2.51	0.49
1:A:494:ASN:HD21	1:A:496:PHE:HD1	1.59	0.49
1:B:473:PHE:CE2	1:B:638[B]:ILE:HG12	2.48	0.49
1:B:423:ILE:HD11	1:B:633:ARG:HB2	1.94	0.49
1:B:472:ASN:OD1	1:B:495:THR:HG23	2.12	0.48
1:A:488:PRO:O	1:A:490:VAL:HG23	2.13	0.48
1:B:572:ILE:HG22	1:B:573:ASP:N	2.29	0.47
1:B:591:SER:HA	1:B:596:GLN:NE2	2.29	0.47
1:A:533:HIS:CD2	1:A:535:CYS:SG	3.08	0.47
1:B:518:VAL:HG13	1:B:524:LEU:HD11	1.97	0.47
1:B:449[B]:ARG:HH11	1:B:449[B]:ARG:CB	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LYS:HD3	1:A:485:LYS:HA	1.57	0.46
1:B:585:GLN:N	1:B:585:GLN:OE1	2.49	0.46
1:B:550:ASP:OD2	1:B:554:GLY:HA3	2.14	0.46
1:B:452:ILE:HG21	1:B:638[B]:ILE:CD1	2.46	0.45
1:A:575:LYS:HA	1:A:575:LYS:HD3	1.30	0.45
1:A:597:GLN:HE22	1:A:603:CYS:HB3	1.82	0.45
1:B:522:ASP:OD1	1:B:542[B]:ARG:HG3	2.17	0.45
1:A:448:PHE:O	1:A:449:ARG:CB	2.64	0.45
1:A:575:LYS:O	1:A:577:LYS:CG	2.65	0.45
2:B:1647:GOL:O3	2:B:1647:GOL:O1	2.29	0.45
1:B:467:ASN:OD1	1:B:467:ASN:C	2.54	0.45
1:B:544:LYS:HE2	1:B:544:LYS:HB3	1.84	0.45
1:B:448:PHE:O	1:B:450:LEU:HG	2.17	0.45
1:B:449[B]:ARG:NH1	1:B:449[B]:ARG:CG	2.36	0.44
1:B:526:VAL:HG12	1:B:528:ILE:HD13	1.99	0.44
1:B:510:LYS:HG2	1:B:573:ASP:OD2	2.17	0.44
1:B:560:CYS:HB2	4:B:2016:HOH:O	2.17	0.44
1:B:560:CYS:HB2	1:B:586:LEU:HB3	2.00	0.44
1:A:540:ASP:CG	1:A:543:LYS:HG3	2.39	0.43
1:A:543:LYS:O	1:A:544:LYS:HB2	2.18	0.43
1:B:571:SER:N	1:B:572:ILE:N	2.66	0.43
1:B:452:ILE:HG21	1:B:638[B]:ILE:HD12	2.01	0.43
1:B:443:VAL:HG13	1:B:451:THR:HG23	2.00	0.43
1:B:565:GLN:HG3	1:B:569:GLN:NE2	2.34	0.43
1:B:521:VAL:O	1:B:541:PHE:HD2	2.02	0.43
1:A:512:TRP:HD1	1:A:512:TRP:N	2.15	0.42
1:B:459:THR:HB	1:B:465[A]:TRP:O	2.20	0.42
1:A:578:GLU:HG2	1:A:578:GLU:H	1.59	0.42
1:B:498:PHE:CD2	1:B:528:ILE:HG23	2.54	0.42
1:A:420:PHE:HB3	1:A:629:TYR:OH	2.20	0.42
1:B:550:ASP:O	1:B:594:ILE:HD11	2.20	0.42
1:A:545:ASN:HB2	1:A:585:GLN:O	2.20	0.42
1:A:575:LYS:HZ2	1:A:575:LYS:HG2	1.59	0.42
1:B:567:LEU:O	1:B:571:SER:N	2.53	0.42
1:B:599:ASN:HD22	1:B:599:ASN:N	2.18	0.41
1:B:497:PHE:CD2	1:B:498:PHE:N	2.88	0.41
1:A:459:THR:HB	1:A:465[A]:TRP:O	2.20	0.41
1:A:465[B]:TRP:CZ3	1:A:532:VAL:O	2.74	0.41
1:B:546:ILE:HD11	1:B:560:CYS:CB	2.30	0.41
1:A:433:ASN:O	1:A:436:ARG:HB2	2.21	0.41
1:B:514:LYS:HG3	1:B:515:LYS:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:TYR:N	1:B:549:TYR:CD2	2.89	0.40

All (2) 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)
1:A:430:GLU:OE1	3:B:1651:CO:CO[3_654]	1.61	0.59
1:A:430:GLU:OE1	1:B:430:GLU:OE1[3_654]	2.11	0.09

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	229/230 (100%)	217 (95%)	11 (5%)	1 (0%)	34	41
1	B	232/230 (101%)	207 (89%)	22 (10%)	3 (1%)	12	11
All	All	461/460 (100%)	424 (92%)	33 (7%)	4 (1%)	22	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	ASN
1	B	449[A]	ARG
1	B	449[B]	ARG
1	B	553	GLY

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	206/213 (97%)	181 (88%)	25 (12%)	5	4
1	B	206/213 (97%)	186 (90%)	20 (10%)	8	8
All	All	412/426 (97%)	367 (89%)	45 (11%)	6	6

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418	ASP
1	A	437	ASN
1	A	444	LEU
1	A	448	PHE
1	A	455	LYS
1	A	461	ASN
1	A	483	LYS
1	A	484	GLU
1	A	485	LYS
1	A	494	ASN
1	A	499	THR
1	A	515	LYS
1	A	518	VAL
1	A	555	ILE
1	A	558	GLU
1	A	571	SER
1	A	572	ILE
1	A	573	ASP
1	A	575	LYS
1	A	582	ASN
1	A	592	GLN
1	A	594	ILE
1	A	616[A]	LYS
1	A	616[B]	LYS
1	A	629	TYR
1	B	419	GLU
1	B	479	MET
1	B	487	LEU
1	B	494	ASN
1	B	499	THR
1	B	502	LYS
1	B	510	LYS
1	B	522	ASP

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Mol	Chain	Res	Type
1	B	544	LYS
1	B	546	ILE
1	B	547	THR
1	B	558	GLU
1	B	586	LEU
1	B	589	LYS
1	B	591	SER
1	B	592	GLN
1	B	616	LYS
1	B	618[A]	ARG
1	B	618[B]	ARG
1	B	621	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	433	ASN
1	A	440	GLN
1	A	461	ASN
1	A	597	GLN
1	B	529	HIS
1	B	569	GLN
1	B	582	ASN
1	B	597	GLN
1	B	599	ASN
1	B	621	ASN

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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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
2	GOL	A	1646	-	5,5,5	0.37	0	5,5,5	0.40	0
2	GOL	B	1648	-	5,5,5	0.29	0	5,5,5	0.52	0
2	GOL	A	1648	-	5,5,5	0.45	0	5,5,5	0.18	0
2	GOL	A	1645	-	5,5,5	0.38	0	5,5,5	0.41	0
2	GOL	B	1645	-	5,5,5	0.40	0	5,5,5	0.44	0
2	GOL	B	1646	-	5,5,5	0.41	0	5,5,5	0.36	0
2	GOL	B	1649	-	5,5,5	0.46	0	5,5,5	0.11	0
2	GOL	B	1650	-	5,5,5	0.31	0	5,5,5	0.38	0
2	GOL	A	1647	-	5,5,5	0.47	0	5,5,5	0.45	0
2	GOL	B	1647	-	5,5,5	0.35	0	5,5,5	0.44	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
2	GOL	A	1646	-	-	3/4/4/4	-
2	GOL	B	1648	-	-	2/4/4/4	-
2	GOL	A	1648	-	-	2/4/4/4	-
2	GOL	A	1645	-	-	4/4/4/4	-
2	GOL	B	1645	-	-	2/4/4/4	-
2	GOL	B	1646	-	-	2/4/4/4	-
2	GOL	B	1649	-	-	2/4/4/4	-
2	GOL	B	1650	-	-	2/4/4/4	-
2	GOL	A	1647	-	-	4/4/4/4	-
2	GOL	B	1647	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1646	GOL	C1-C2-C3-O3
2	A	1646	GOL	O2-C2-C3-O3
2	A	1648	GOL	C1-C2-C3-O3
2	A	1645	GOL	C1-C2-C3-O3
2	A	1645	GOL	O2-C2-C3-O3
2	B	1645	GOL	C1-C2-C3-O3
2	B	1646	GOL	C1-C2-C3-O3
2	B	1646	GOL	O2-C2-C3-O3
2	B	1649	GOL	C1-C2-C3-O3
2	B	1649	GOL	O2-C2-C3-O3
2	B	1650	GOL	O1-C1-C2-C3
2	A	1647	GOL	O1-C1-C2-C3
2	A	1647	GOL	C1-C2-C3-O3
2	B	1645	GOL	O2-C2-C3-O3
2	A	1645	GOL	O1-C1-C2-C3
2	A	1648	GOL	O2-C2-C3-O3
2	A	1645	GOL	O1-C1-C2-O2
2	B	1650	GOL	O1-C1-C2-O2
2	A	1647	GOL	O1-C1-C2-O2
2	A	1647	GOL	O2-C2-C3-O3
2	A	1646	GOL	O1-C1-C2-O2
2	B	1648	GOL	O2-C2-C3-O3
2	B	1648	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1645	GOL	1	0
2	B	1646	GOL	2	0
2	B	1647	GOL	2	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	227/230 (98%)	0.34	10 (4%) 34 32	24, 45, 71, 89	0
1	B	226/230 (98%)	0.54	22 (9%) 7 5	28, 60, 96, 100	0
All	All	453/460 (98%)	0.44	32 (7%) 16 12	24, 50, 85, 100	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	576	ARG	6.5
1	B	582	ASN	5.0
1	B	584	TRP	4.9
1	B	436	ARG	4.7
1	B	437	ASN	4.6
1	B	579	PHE	4.3
1	B	435	PHE	3.8
1	A	516	VAL	3.8
1	B	583	GLY	3.8
1	B	588	SER	3.6
1	B	586	LEU	3.6
1	B	542[A]	ARG	3.5
1	B	520	SER	3.5
1	B	576	ARG	3.5
1	A	418	ASP	3.3
1	B	564	LEU	3.3
1	A	572	ILE	2.9
1	B	563	LEU	2.9
1	A	583	GLY	2.8
1	B	541	PHE	2.6
1	B	585	GLN	2.6
1	A	573	ASP	2.5
1	B	587	PHE	2.5
1	A	578	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	523	ILE	2.4
1	A	515	LYS	2.4
1	B	578	GLU	2.4
1	B	547	THR	2.3
1	A	511	ARG	2.2
1	B	580	ASP	2.1
1	B	519	PHE	2.0
1	A	486	GLY	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 carbohydrates in this entry.

6.4 Ligands ⓘ

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
2	GOL	B	1645	6/6	0.77	0.34	79,82,84,84	0
2	GOL	A	1648	6/6	0.79	0.17	63,67,74,75	0
2	GOL	B	1646	6/6	0.80	0.20	76,77,81,87	0
2	GOL	B	1648	6/6	0.81	0.24	63,65,73,77	0
2	GOL	B	1647	6/6	0.81	0.28	50,59,66,72	0
2	GOL	A	1646	6/6	0.82	0.19	65,67,73,76	0
2	GOL	A	1647	6/6	0.83	0.33	68,77,82,85	0
2	GOL	A	1645	6/6	0.83	0.22	42,52,57,71	0
2	GOL	B	1650	6/6	0.89	0.15	68,75,79,83	0
2	GOL	B	1649	6/6	0.90	0.13	57,69,70,73	0
3	CO	B	1651	1/1	1.00	0.18	11,11,11,11	1

6.5 Other polymers ⓘ

There are no such residues in this entry.