



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:38 PM UTC

PDB ID : 2XPH / pdb_00002xph
Title : Crystal structure of human SENP1 with the bound cobalt
Authors : Rimsa, V.; Eadsforth, T.; Hay, R.T.; Hunter, W.N.
Deposited on : 2010-08-26
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

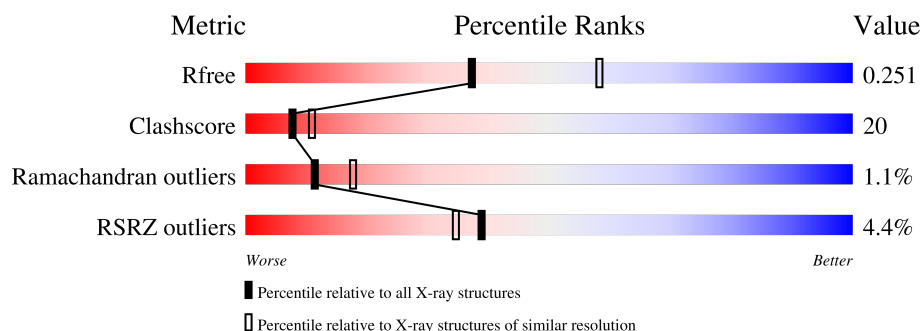
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	238	4% 58% 33% 5% 5%
1	B	238	5% 65% 28% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3978 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	78	4	0
			1928	1235	333	346	14			
1	B	226	Total	C	N	O	S	59	7	0
			1943	1251	338	340	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	407	GLY	-	expression tag	UNP Q9P0U3
A	408	ALA	-	expression tag	UNP Q9P0U3
A	409	MET	-	expression tag	UNP Q9P0U3
A	410	ALA	-	expression tag	UNP Q9P0U3
A	411	ASP	-	expression tag	UNP Q9P0U3
A	412	ILE	-	expression tag	UNP Q9P0U3
A	413	GLY	-	expression tag	UNP Q9P0U3
A	414	SER	-	expression tag	UNP Q9P0U3
B	407	GLY	-	expression tag	UNP Q9P0U3
B	408	ALA	-	expression tag	UNP Q9P0U3
B	409	MET	-	expression tag	UNP Q9P0U3
B	410	ALA	-	expression tag	UNP Q9P0U3
B	411	ASP	-	expression tag	UNP Q9P0U3
B	412	ILE	-	expression tag	UNP Q9P0U3
B	413	GLY	-	expression tag	UNP Q9P0U3
B	414	SER	-	expression tag	UNP Q9P0U3

- Molecule 2 is GLYCEROL (CCD ID: 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		
2	A	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 (CCD ID: CO) (formula: Co).

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

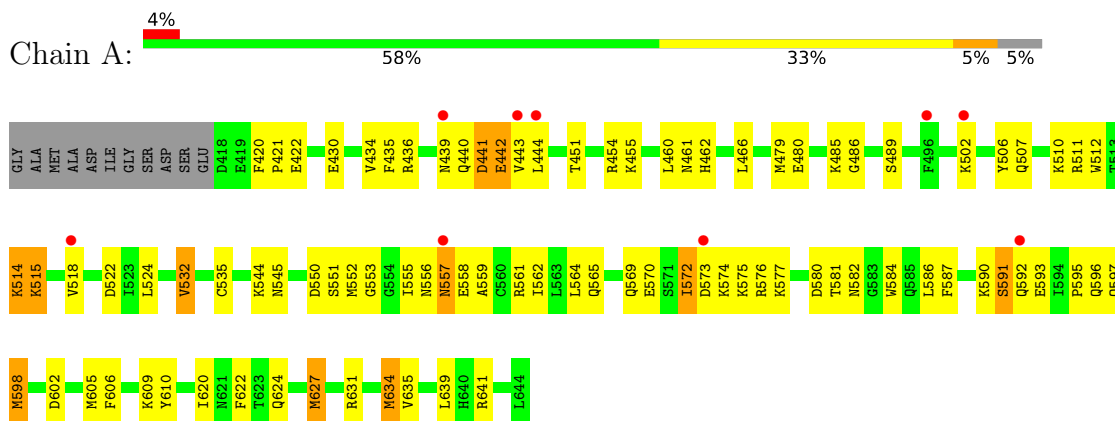
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	29	Total	O	0	0
			29	29		

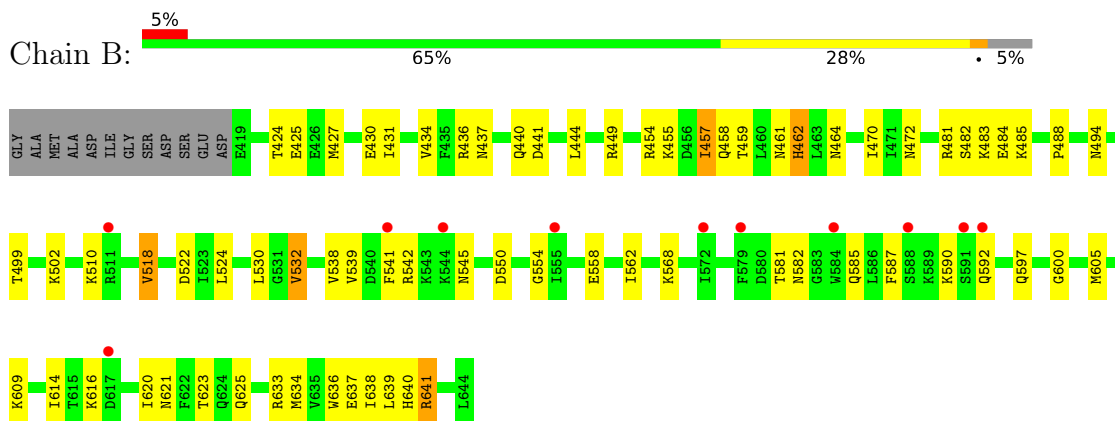
3 Residue-property plots

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: 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	71.17Å 71.17Å 199.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	66.66 – 2.40 66.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (66.66-2.40) 99.7 (66.66-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.227 , 0.313 (Not available) , 0.251	Depositor DCC
R_{free} test set	1193 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3978	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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, 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	1.17	6/1980 (0.3%)	1.32	24/2660 (0.9%)
1	B	1.30	11/2009 (0.5%)	1.61	22/2699 (0.8%)
All	All	1.24	17/3989 (0.4%)	1.48	46/5359 (0.9%)

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 (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	514	LYS	CA-CB	-20.99	1.19	1.53
1	B	641[A]	ARG	C-N	-20.11	1.07	1.33
1	B	641[B]	ARG	C-N	-20.11	1.07	1.33
1	A	515	LYS	CD-CE	-15.67	1.05	1.52
1	B	441	ASP	CA-CB	-14.71	1.27	1.53
1	B	485	LYS	CA-CB	-12.85	1.31	1.53
1	B	641[A]	ARG	CA-C	-9.84	1.41	1.53
1	B	641[B]	ARG	CA-C	-9.84	1.41	1.53
1	B	436	ARG	CA-CB	-9.26	1.41	1.53
1	A	511	ARG	CA-CB	-8.75	1.39	1.53
1	A	502	LYS	CG-CD	-8.51	1.26	1.52
1	B	641[A]	ARG	N-CA	8.33	1.58	1.46
1	B	641[B]	ARG	N-CA	8.33	1.58	1.46
1	B	510	LYS	CB-CG	-5.83	1.34	1.52
1	A	515	LYS	CE-NZ	-5.71	1.32	1.49
1	B	457	ILE	CA-CB	5.25	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	515	LYS	CG-CD	-5.21	1.36	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	641[A]	ARG	CA-C-O	-29.70	86.90	121.65
1	B	641[B]	ARG	CA-C-O	-29.70	86.90	121.65
1	B	641[A]	ARG	O-C-N	-18.04	100.93	122.58
1	B	641[B]	ARG	O-C-N	-18.04	100.93	122.58
1	B	485	LYS	N-CA-CB	-16.70	85.43	109.97
1	A	515	LYS	CG-CD-CE	14.86	145.48	111.30
1	A	514	LYS	N-CA-CB	14.39	132.57	109.69
1	B	641[A]	ARG	CA-C-N	13.53	143.24	121.86
1	B	641[A]	ARG	C-N-CA	13.53	143.24	121.86
1	B	641[B]	ARG	CA-C-N	13.53	143.24	121.86
1	B	641[B]	ARG	C-N-CA	13.53	143.24	121.86
1	B	641[A]	ARG	CB-CA-C	12.48	128.59	111.86
1	B	641[B]	ARG	CB-CA-C	12.48	128.59	111.86
1	A	502	LYS	CB-CG-CD	11.98	138.85	111.30
1	A	422	GLU	CA-CB-CG	9.78	133.66	114.10
1	A	572	ILE	CB-CA-C	9.63	127.09	111.29
1	B	510	LYS	CA-CB-CG	8.53	131.16	114.10
1	A	535	CYS	N-CA-C	-8.26	98.05	108.45
1	A	511	ARG	N-CA-CB	7.99	121.99	110.16
1	B	441	ASP	N-CA-CB	7.61	123.02	110.39
1	B	462	HIS	N-CA-C	7.24	119.79	111.11
1	A	422	GLU	CB-CG-CD	7.18	124.81	112.60
1	A	441	ASP	N-CA-C	-6.88	106.08	114.75
1	A	532	VAL	N-CA-C	-6.84	106.46	113.10
1	A	502	LYS	CG-CD-CE	6.78	126.88	111.30
1	A	442	GLU	N-CA-C	-6.55	100.95	110.64
1	B	485	LYS	CA-CB-CG	6.55	127.20	114.10
1	A	572	ILE	CA-CB-CG1	6.52	121.49	110.40
1	B	641[A]	ARG	N-CA-C	-6.36	102.61	111.52
1	B	641[B]	ARG	N-CA-C	-6.36	102.61	111.52
1	A	634	MET	N-CA-C	-6.32	104.47	111.36
1	B	532	VAL	CB-CA-C	-6.27	104.98	112.19
1	A	598	MET	N-CA-C	-6.21	105.19	114.64
1	A	587	PHE	N-CA-C	6.13	118.50	109.24
1	A	455	LYS	CA-CB-CG	-6.10	101.90	114.10
1	A	627	MET	CA-C-N	-5.86	112.97	119.19
1	A	627	MET	C-N-CA	-5.86	112.97	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	LYS	CA-CB-CG	-5.84	102.42	114.10
1	A	506	TYR	N-CA-C	5.83	118.38	111.33
1	B	485	LYS	CB-CA-C	5.58	119.19	109.65
1	A	510	LYS	N-CA-CB	-5.53	100.22	110.18
1	B	462	HIS	CA-C-N	-5.51	114.42	122.86
1	B	462	HIS	C-N-CA	-5.51	114.42	122.86
1	A	609	LYS	CB-CG-CD	5.42	123.77	111.30
1	A	444	LEU	N-CA-C	5.38	118.94	112.38
1	B	582	ASN	N-CA-C	5.20	116.63	109.15

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	641[A]	ARG	Mainchain
1	B	641[B]	ARG	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	1928	0	1926	82	1
1	B	1943	0	1963	68	1
2	A	30	0	40	3	0
2	B	6	0	8	1	0
3	B	1	0	0	0	0
4	A	41	0	0	4	0
4	B	29	0	0	0	0
All	All	3978	0	3937	149	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 20.

All (149) 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:449[B]:ARG:HB3	1:B:449[B]:ARG:NH1	1.67	1.10
1:B:522:ASP:HB3	1:B:542:ARG:CD	1.83	1.08
1:B:449[B]:ARG:HB3	1:B:449[B]:ARG:HH11	0.92	1.07
1:B:522:ASP:CB	1:B:542:ARG:HD3	1.84	1.07
1:A:436[B]:ARG:HH11	1:A:436[B]:ARG:CG	1.71	1.02
1:A:436[B]:ARG:HH11	1:A:436[B]:ARG:HG2	1.21	1.02
1:B:449[B]:ARG:HH11	1:B:449[B]:ARG:CB	1.73	1.00
1:A:590:LYS:O	1:A:591:SER:HB3	1.62	0.94
1:B:449[B]:ARG:NH1	1:B:449[B]:ARG:CB	2.30	0.94
1:B:545:ASN:ND2	1:B:587:PHE:HE1	1.65	0.93
1:B:522:ASP:HB3	1:B:542:ARG:HD3	0.93	0.90
1:B:545:ASN:ND2	1:B:587:PHE:CE1	2.39	0.90
1:A:590:LYS:O	1:A:591:SER:CB	2.20	0.88
1:A:436[B]:ARG:NH1	1:A:436[B]:ARG:HB3	1.91	0.84
1:B:488:PRO:HB3	1:B:542:ARG:NH1	1.96	0.81
1:B:605:MET:HE1	1:B:634:MET:HE3	1.63	0.81
1:A:436[B]:ARG:HH11	1:A:436[B]:ARG:CB	1.96	0.79
1:B:545:ASN:ND2	1:B:585:GLN:HB2	1.97	0.79
1:A:436[B]:ARG:HG2	1:A:436[B]:ARG:NH1	1.99	0.76
1:A:434:VAL:HG21	1:A:639:LEU:HD11	1.68	0.76
1:A:507[B]:GLN:NE2	1:A:507[B]:GLN:H	1.84	0.76
1:A:479:MET:CE	4:A:2015:HOH:O	2.35	0.73
1:A:441:ASP:O	1:A:442:GLU:C	2.32	0.71
1:A:436[B]:ARG:NH1	1:A:436[B]:ARG:CB	2.52	0.71
1:B:621:ASN:H	1:B:621:ASN:HD22	1.37	0.71
1:A:479:MET:HE3	4:A:2015:HOH:O	1.91	0.70
1:B:545:ASN:HD21	1:B:587:PHE:HE1	1.38	0.70
1:A:485:LYS:HD3	1:A:486:GLY:H	1.58	0.69
1:B:636:TRP:CE2	1:B:640:HIS:CE1	2.81	0.67
1:A:485:LYS:CD	1:A:486:GLY:H	2.07	0.67
1:B:524:LEU:HB2	1:B:539:VAL:HB	1.78	0.66
1:A:592:GLN:HG2	1:A:593:GLU:N	2.10	0.66
1:A:592:GLN:OE1	1:A:592:GLN:C	2.40	0.64
1:B:481:ARG:NH2	1:B:616:LYS:HG3	2.13	0.63
1:A:627:MET:O	1:A:631:ARG:HG3	1.97	0.63
1:A:602:ASP:O	1:A:606:PHE:HD1	1.83	0.62
1:A:565:GLN:O	1:A:569:GLN:HG3	2.01	0.60
1:B:449[A]:ARG:HG2	1:B:449[A]:ARG:HH11	1.66	0.59
1:B:434:VAL:HG11	1:B:639:LEU:HD11	1.84	0.59
1:A:439:ASN:C	1:A:441:ASP:H	2.11	0.59
1:B:558:GLU:O	1:B:562:ILE:HG13	2.02	0.59
1:A:435:PHE:CZ	1:A:635:VAL:HG21	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:SER:C	1:B:484:GLU:H	2.11	0.58
1:B:609:LYS:HE3	1:B:609:LYS:HA	1.87	0.57
1:B:621:ASN:H	1:B:621:ASN:ND2	2.02	0.57
1:B:444:LEU:HD11	1:B:454:ARG:HA	1.87	0.56
1:A:553:GLY:HA3	1:A:591:SER:HB2	1.88	0.56
1:A:558:GLU:O	1:A:562:ILE:HG13	2.06	0.56
1:A:480[A]:GLU:OE1	1:A:641:ARG:NH1	2.39	0.56
1:B:545:ASN:HD21	1:B:585:GLN:HB2	1.68	0.55
1:A:545:ASN:OD1	1:A:545:ASN:C	2.50	0.55
1:B:449[B]:ARG:NH1	1:B:449[B]:ARG:HB2	2.18	0.55
1:A:580:ASP:OD1	1:A:582:ASN:HB2	2.06	0.55
1:A:595:PRO:O	1:A:610:TYR:OH	2.24	0.54
1:B:634:MET:O	1:B:638[B]:ILE:HG22	2.07	0.54
1:B:449[A]:ARG:HG2	1:B:449[A]:ARG:NH1	2.23	0.54
1:B:427:MET:HE3	1:B:636:TRP:CE2	2.42	0.54
1:A:552:MET:HE1	1:B:530:LEU:HD22	1.90	0.54
1:B:568:LYS:HE2	1:B:581:THR:HG21	1.90	0.54
1:B:424:THR:OG1	1:B:427:MET:HG3	2.08	0.53
1:A:461:ASN:HD22	1:A:462:HIS:H	1.55	0.53
1:B:488:PRO:HB3	1:B:542:ARG:HH11	1.71	0.53
1:A:592:GLN:HG2	1:A:593:GLU:H	1.74	0.53
1:B:636:TRP:NE1	1:B:640:HIS:CE1	2.77	0.53
1:A:553:GLY:CA	1:A:591:SER:HB2	2.39	0.52
1:A:564:LEU:HD22	1:A:586:LEU:HD21	1.91	0.52
1:A:598:MET:HB2	1:A:624:GLN:HG2	1.92	0.51
1:A:575:LYS:C	1:A:577:LYS:H	2.18	0.51
1:A:592:GLN:O	1:A:593:GLU:HB2	2.11	0.51
1:B:623:THR:OG1	1:B:625[A]:GLN:HG2	2.11	0.50
1:B:633:ARG:O	1:B:637:GLU:HG3	2.12	0.50
1:B:621:ASN:HD22	1:B:621:ASN:N	2.02	0.50
1:A:556:ASN:O	1:A:556:ASN:OD1	2.30	0.49
1:B:502:LYS:HG3	1:B:562:ILE:HD13	1.94	0.49
1:A:480[A]:GLU:CD	1:A:641:ARG:HH12	2.20	0.49
1:B:482:SER:C	1:B:484:GLU:N	2.70	0.49
1:A:514:LYS:O	1:A:515:LYS:HG3	2.13	0.49
1:A:518:VAL:HG22	1:A:524:LEU:CD2	2.42	0.49
1:A:592:GLN:OE1	1:A:592:GLN:O	2.29	0.49
1:A:434:VAL:C	1:A:436[B]:ARG:H	2.19	0.49
1:A:556:ASN:OD1	1:A:559:ALA:N	2.31	0.49
1:B:482:SER:O	1:B:484:GLU:N	2.43	0.49
1:B:518:VAL:O	1:B:541:PHE:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:LYS:O	1:A:577:LYS:HG3	2.13	0.49
1:A:557:ASN:O	1:A:561:ARG:HG3	2.13	0.48
1:A:555:ILE:HG22	1:A:556:ASN:N	2.26	0.48
1:B:592:GLN:NE2	1:B:592:GLN:H	2.11	0.48
1:B:449[B]:ARG:CB	1:B:449[B]:ARG:CZ	2.92	0.48
1:B:454:ARG:O	1:B:458:GLN:HG2	2.14	0.48
1:A:555:ILE:CG2	1:A:556:ASN:N	2.77	0.48
1:A:591:SER:HA	1:A:596:GLN:NE2	2.28	0.48
1:B:488:PRO:HB3	1:B:542:ARG:HH12	1.73	0.48
1:B:605:MET:O	1:B:609:LYS:HG2	2.14	0.48
1:B:454:ARG:HG2	1:B:458:GLN:HE21	1.79	0.48
1:A:434:VAL:C	1:A:436[A]:ARG:H	2.20	0.47
1:A:551:SER:O	1:A:597:GLN:HG2	2.14	0.47
1:B:431:ILE:O	1:B:434:VAL:HG22	2.14	0.47
1:A:480[A]:GLU:OE2	1:A:641:ARG:NH1	2.48	0.47
1:A:532:VAL:HG13	1:B:499:THR:HB	1.97	0.46
2:A:1645:GOL:H12	1:B:532:VAL:HG11	1.96	0.46
1:A:507[B]:GLN:H	1:A:507[B]:GLN:HE21	1.59	0.46
1:B:590:LYS:C	1:B:592:GLN:N	2.73	0.46
1:A:443:VAL:HG13	1:A:451:THR:HG23	1.98	0.46
1:B:464:ASN:HD21	2:B:1645:GOL:H2	1.81	0.45
1:B:518:VAL:O	1:B:518:VAL:HG13	2.17	0.45
1:A:480[B]:GLU:HA	1:A:480[B]:GLU:OE1	2.17	0.45
1:A:460:LEU:HD23	1:A:466:LEU:HD11	1.98	0.44
1:B:620:ILE:N	1:B:620:ILE:HD12	2.32	0.44
1:A:480[A]:GLU:CD	1:A:641:ARG:NH1	2.75	0.44
1:B:542:ARG:HE	1:B:542:ARG:HB2	1.50	0.44
1:A:436[B]:ARG:HB3	1:A:436[B]:ARG:CZ	2.48	0.44
1:A:441:ASP:O	1:A:443:VAL:N	2.51	0.44
1:A:489:SER:OG	1:A:522:ASP:OD2	2.35	0.44
1:A:592:GLN:CG	1:A:593:GLU:N	2.78	0.44
1:A:479:MET:HE1	4:A:2015:HOH:O	2.07	0.43
1:B:440:GLN:HB3	1:B:455:LYS:HB2	2.00	0.43
1:A:485:LYS:HD3	1:A:486:GLY:N	2.29	0.43
1:B:550:ASP:OD2	1:B:554:GLY:HA3	2.17	0.43
1:A:420:PHE:O	1:A:421:PRO:C	2.60	0.43
1:A:555:ILE:O	2:A:1645:GOL:H11	2.19	0.43
1:B:425:GLU:H	1:B:425:GLU:CD	2.26	0.43
1:B:461:ASN:OD1	1:B:462:HIS:N	2.49	0.43
1:B:597:GLN:NE2	1:B:600:GLY:HA2	2.34	0.43
1:A:550:ASP:OD1	1:A:552:MET:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:GLU:O	1:A:573:ASP:O	2.36	0.43
1:A:544:LYS:O	1:A:584:TRP:HA	2.19	0.43
1:B:472:ASN:OD1	1:B:494:ASN:HB2	2.18	0.43
1:A:434:VAL:CG2	1:A:639:LEU:HD11	2.44	0.42
1:A:572:ILE:O	1:A:576:ARG:HA	2.18	0.42
1:A:439:ASN:C	1:A:441:ASP:N	2.77	0.42
1:A:575:LYS:C	1:A:577:LYS:N	2.78	0.42
1:B:538:VAL:HG21	1:B:614:ILE:HD13	2.02	0.41
2:A:1648:GOL:H11	4:A:2003:HOH:O	2.20	0.41
1:B:592:GLN:H	1:B:592:GLN:HE21	1.66	0.41
1:A:582:ASN:HD22	1:A:582:ASN:HA	1.65	0.41
1:A:605:MET:HE1	1:A:634:MET:HE3	2.01	0.41
1:A:620:ILE:HG23	1:A:622:PHE:CE2	2.55	0.41
1:A:507[B]:GLN:NE2	1:A:507[B]:GLN:N	2.60	0.41
1:A:518:VAL:HG22	1:A:524:LEU:HD21	2.02	0.41
1:A:485:LYS:CG	1:A:486:GLY:H	2.34	0.41
1:B:590:LYS:C	1:B:592:GLN:H	2.28	0.41
1:A:512:TRP:CD1	1:A:512:TRP:N	2.88	0.40
1:A:564:LEU:HD11	1:A:581:THR:HG22	2.02	0.40
1:B:457:ILE:HD13	1:B:457:ILE:HA	1.96	0.40
1:A:440:GLN:HG2	1:A:454:ARG:HE	1.86	0.40
1:A:512:TRP:CD1	1:A:512:TRP:H	2.39	0.40
1:B:437:ASN:HD22	1:B:437:ASN:C	2.27	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)
1:A:430:GLU:OE1	1:B:430:GLU:OE1[3_664]	2.08	0.12

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	229/238 (96%)	199 (87%)	27 (12%)	3 (1%)	9	14
1	B	231/238 (97%)	209 (90%)	20 (9%)	2 (1%)	14	22
All	All	460/476 (97%)	408 (89%)	47 (10%)	5 (1%)	11	18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	574	LYS
1	A	591	SER
1	A	557	ASN
1	B	483	LYS
1	B	518	VAL

5.3.2 Protein sidechains [i](#)

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

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](#)

Of 7 ligands modelled in this entry, 1 is 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
2	GOL	A	1648	-	5,5,5	0.45	0	5,5,5	0.39	0
2	GOL	A	1647	-	5,5,5	0.48	0	5,5,5	0.54	0
2	GOL	A	1645	-	5,5,5	0.41	0	5,5,5	0.72	0
2	GOL	A	1646	-	5,5,5	0.35	0	5,5,5	0.69	0
2	GOL	A	1649	-	5,5,5	0.30	0	5,5,5	0.63	0
2	GOL	B	1645	-	5,5,5	0.23	0	5,5,5	0.33	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	1648	-	-	2/4/4/4	-
2	GOL	A	1647	-	-	4/4/4/4	-
2	GOL	A	1645	-	-	4/4/4/4	-
2	GOL	A	1646	-	-	4/4/4/4	-
2	GOL	A	1649	-	-	1/4/4/4	-
2	GOL	B	1645	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

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

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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1648	GOL	1	0
2	A	1645	GOL	2	0
2	B	1645	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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	641:ARG	C	642:LYS	N	1.07

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	227/238 (95%)	0.25	9 (3%) 42 38	21, 54, 87, 99	22 (9%)
1	B	226/238 (94%)	0.46	11 (4%) 35 31	21, 61, 92, 100	20 (8%)
All	All	453/476 (95%)	0.35	20 (4%) 39 34	21, 56, 90, 100	42 (9%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	557	ASN	3.6
1	B	579	PHE	3.5
1	B	617	ASP	2.9
1	A	444	LEU	2.9
1	B	544	LYS	2.8
1	A	443	VAL	2.8
1	B	555	ILE	2.5
1	B	588	SER	2.5
1	B	584	TRP	2.4
1	B	591	SER	2.4
1	A	573	ASP	2.4
1	B	541	PHE	2.3
1	B	592	GLN	2.3
1	A	592	GLN	2.3
1	A	518	VAL	2.3
1	B	511	ARG	2.3
1	A	496	PHE	2.2
1	B	572	ILE	2.2
1	A	502	LYS	2.1
1	A	439	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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
2	GOL	A	1645	6/6	0.68	0.15	65,68,71,74	0
2	GOL	A	1648	6/6	0.69	0.14	67,80,81,83	0
2	GOL	A	1646	6/6	0.84	0.13	69,72,76,81	0
2	GOL	A	1647	6/6	0.85	0.12	52,72,78,78	0
2	GOL	A	1649	6/6	0.88	0.16	85,86,92,93	0
2	GOL	B	1645	6/6	0.88	0.12	60,64,65,70	0
3	CO	B	1646	1/1	0.98	0.08	16,16,16,16	1

6.5 Other polymers [i](#)

There are no such residues in this entry.