



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:36 AM GMT

PDB ID : 2XPH
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

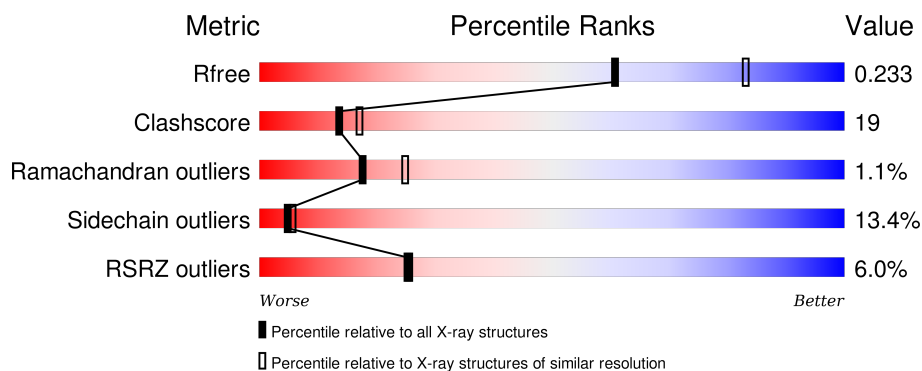
1 Overall quality at a glance ⓘ

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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>5%</div> <div>54%</div> <div>31%</div> <div>10%</div> <div>• 5%</div> </div>
1	B	238	<div> <div>7%</div> <div>64%</div> <div>26%</div> <div>5%</div> <div>5%</div> </div>

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
2	GOL	A	1645	-	-	-	X
2	GOL	A	1649	-	-	-	X
3	CO	B	1646	-	-	-	X

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 (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

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

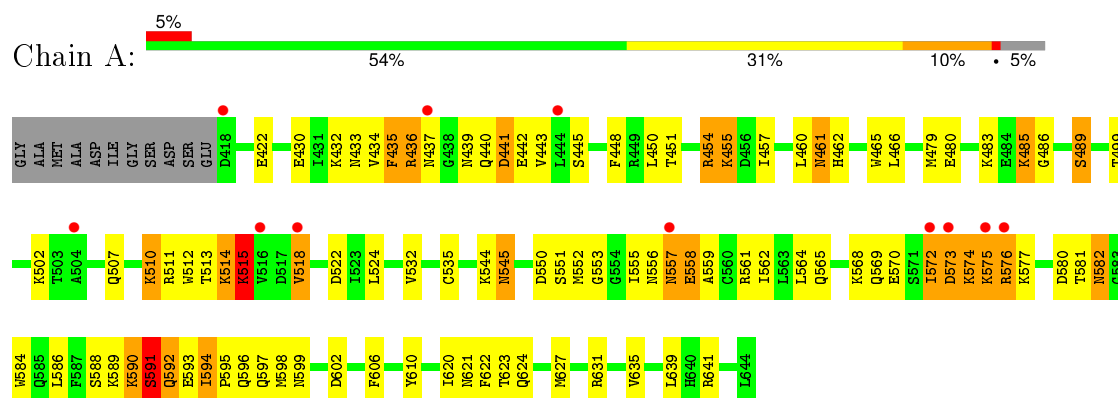
- Molecule 4 is water.

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

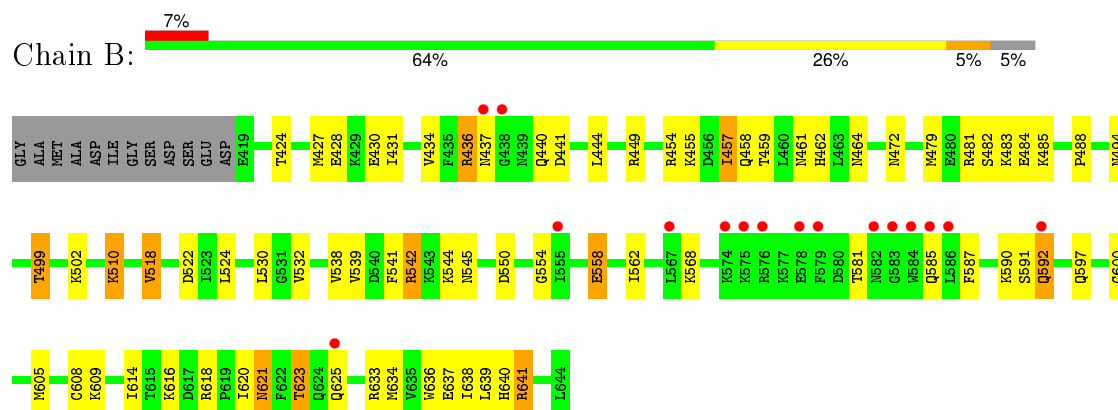
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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	71.17Å 71.17Å 199.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	66.66 – 2.40 38.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (66.66-2.40) 99.7 (38.83-2.40)	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 0.231 , 0.233	Depositor DCC
R_{free} test set	1193 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.3	EDS
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 23754 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.00	5/1980 (0.3%)	0.96	9/2660 (0.3%)
1	B	0.99	9/2009 (0.4%)	1.19	15/2699 (0.6%)
All	All	1.00	14/3989 (0.4%)	1.08	24/5359 (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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	515	LYS	CD-CE	-18.33	1.05	1.51
1	A	514	LYS	CA-CB	-15.66	1.19	1.53
1	B	441	ASP	CA-CB	-11.90	1.27	1.53
1	B	641[A]	ARG	C-N	-11.40	1.07	1.34
1	B	641[B]	ARG	C-N	-11.40	1.07	1.34
1	B	485	LYS	CA-CB	-10.00	1.31	1.53
1	A	502	LYS	CG-CD	-7.51	1.26	1.52
1	A	515	LYS	CE-NZ	-6.74	1.32	1.49
1	A	511	ARG	CA-CB	-6.63	1.39	1.53
1	B	510	LYS	CB-CG	-6.51	1.34	1.52
1	B	641[A]	ARG	N-CA	6.21	1.58	1.46
1	B	641[B]	ARG	N-CA	6.21	1.58	1.46
1	B	436	ARG	CA-CB	-5.82	1.41	1.53
1	B	608	CYS	CB-SG	-5.63	1.72	1.81

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	641[A]	ARG	CA-C-N	17.24	155.12	117.20
1	B	641[B]	ARG	CA-C-N	17.24	155.12	117.20
1	B	641[A]	ARG	CA-C-O	-15.81	86.90	120.10
1	B	641[B]	ARG	CA-C-O	-15.81	86.90	120.10
1	B	485	LYS	N-CA-CB	-13.98	85.43	110.60
1	B	641[A]	ARG	O-C-N	-13.61	100.93	122.70
1	B	641[B]	ARG	O-C-N	-13.61	100.93	122.70
1	A	514	LYS	N-CA-CB	12.21	132.57	110.60
1	A	515	LYS	CG-CD-CE	11.19	145.48	111.90
1	A	502	LYS	CB-CG-CD	10.48	138.85	111.60
1	B	641[A]	ARG	CB-CA-C	9.35	129.10	110.40
1	B	641[B]	ARG	CB-CA-C	9.35	129.10	110.40
1	A	422	GLU	CA-CB-CG	9.21	133.66	113.40
1	B	641[A]	ARG	C-N-CA	8.62	143.24	121.70
1	B	641[B]	ARG	C-N-CA	8.62	143.24	121.70
1	B	510	LYS	CA-CB-CG	8.07	131.16	113.40
1	A	572	ILE	CB-CA-C	7.74	127.09	111.60
1	B	441	ASP	N-CA-CB	6.90	123.02	110.60
1	A	511	ARG	N-CA-CB	6.33	121.99	110.60
1	B	485	LYS	CA-CB-CG	6.27	127.20	113.40
1	A	510	LYS	N-CA-CB	-5.77	100.22	110.60
1	A	572	ILE	CA-CB-CG1	5.52	121.49	111.00
1	A	455	LYS	CA-CB-CG	-5.23	101.90	113.40
1	B	441	ASP	CB-CG-OD2	5.19	122.97	118.30

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	76	1
1	B	1943	0	1963	63	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	139	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 19.

All (139) 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:NH1	1:B:449[B]:ARG:HB3	1.67	1.10
1:B:522:ASP:HB3	1:B:542:ARG:CD	1.83	1.08
1:B:449[B]:ARG:HH11	1:B:449[B]:ARG:HB3	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:B:449[B]:ARG:NH1	1:B:449[B]:ARG:CB	2.30	0.94
1:A:590:LYS:O	1:A:591:SER:HB3	1.62	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:HB3	1:A:436[B]:ARG:NH1	1.91	0.84
1:B:488:PRO:HB3	1:B:542:ARG:NH1	1.96	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:NH1	1:A:436[B]:ARG:HG2	1.99	0.76
1:A:434:VAL:HG21	1:A:639:LEU:HD11	1.68	0.76
1:A:507[B]:GLN:H	1:A:507[B]:GLN:NE2	1.84	0.76
1:A:479:MET:CE	4:A:2015:HOH:O	2.35	0.73
1:A:436[B]:ARG:CB	1:A:436[B]:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ASP:O	1:A:442:GLU:C	2.32	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: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:592:GLN:C	1:A:592:GLN:OE1	2.40	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
1:B:609:LYS:HE3	1:B:609:LYS:HA	1.87	0.57
1:B:621:ASN:ND2	1:B:621:ASN:H	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: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:A:439:ASN:C	1:A:441:ASP:H	2.11	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:B:482:SER:C	1:B:484:GLU:H	2.11	0.53
1:B:488:PRO:HB3	1:B:542:ARG:HH11	1.71	0.53
1:A:461:ASN:HD22	1:A:462:HIS:H	1.55	0.53
1:B:636:TRP:NE1	1:B:640:HIS:CE1	2.77	0.53
1:A:592:GLN:HG2	1:A:593:GLU:H	1.74	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:592:GLN:O	1:A:593:GLU:HB2	2.11	0.51
1:A:545:ASN:C	1:A:545:ASN:OD1	2.50	0.50
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:N	1:B:621:ASN:HD22	2.02	0.50
1:B:502:LYS:HG3	1:B:562:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ASN:O	1:A:556:ASN:OD1	2.30	0.49
1:A:518:VAL:HG22	1:A:524:LEU:CD2	2.42	0.49
1:A:514:LYS:O	1:A:515:LYS:HG3	2.13	0.49
1:A:592:GLN:O	1:A:592:GLN:OE1	2.29	0.49
1:B:482:SER:O	1:B:484:GLU:N	2.43	0.49
1:A:556:ASN:OD1	1:A:559:ALA:N	2.31	0.49
1:A:594:ILE:O	1:A:594:ILE:CG1	2.59	0.49
1:B:518:VAL:O	1:B:541:PHE:HE2	1.94	0.49
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:CZ	1:B:449[B]:ARG:CB	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:B:431:ILE:O	1:B:434:VAL:HG22	2.14	0.47
1:A:551:SER:O	1:A:597:GLN:HG2	2.14	0.47
1:A:480[A]:GLU:OE2	1:A:641:ARG:NH1	2.48	0.47
1:A:575:LYS:C	1:A:577:LYS:H	2.18	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:HE21	1:A:507[B]:GLN:H	1.59	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:OE1	1:A:480[B]:GLU:HA	2.17	0.45
1:B:482:SER:C	1:B:484:GLU:N	2.70	0.45
1:A:434:VAL:C	1:A:436[B]:ARG:H	2.19	0.44
1:B:634:MET:HB2	1:B:634:MET:HE3	1.83	0.44
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:B:542:ARG:HE	1:B:542:ARG:HB2	1.50	0.44
1:A:436[B]:ARG:CZ	1:A:436[B]:ARG:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:480[A]:GLU:CD	1:A:641:ARG:HH12	2.20	0.43
1:B:550:ASP:OD2	1:B:554:GLY:HA3	2.17	0.43
1:A:555:ILE:O	2:A:1645:GOL:H11	2.19	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:434:VAL:C	1:A:436[A]:ARG:H	2.20	0.43
1:A:550:ASP:OD1	1:A:552:MET:HB2	2.18	0.43
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:B:590:LYS:C	1:B:592:GLN:N	2.73	0.42
1:B:538:VAL:HG21	1:B:614:ILE:HD13	2.02	0.41
1:B:592:GLN:HE21	1:B:592:GLN:H	1.66	0.41
2:A:1648:GOL:H11	4:A:2003:HOH:O	2.20	0.41
1:A:582:ASN:HD22	1:A:582:ASN:HA	1.65	0.41
1:B:621:ASN:ND2	1:B:621:ASN:N	2.67	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:A:512:TRP:N	1:A:512:TRP:CD1	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

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%)	15	21
1	B	231/238 (97%)	209 (90%)	20 (9%)	2 (1%)	21	30
All	All	460/476 (97%)	408 (89%)	47 (10%)	5 (1%)	17	25

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](#)

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	214/217 (99%)	173 (81%)	41 (19%)	2	2
1	B	216/217 (100%)	200 (93%)	16 (7%)	17	26
All	All	430/434 (99%)	373 (87%)	57 (13%)	5	6

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	432	LYS

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Mol	Chain	Res	Type
1	A	433	ASN
1	A	435	PHE
1	A	436[A]	ARG
1	A	436[B]	ARG
1	A	437	ASN
1	A	441	ASP
1	A	445	SER
1	A	448	PHE
1	A	450	LEU
1	A	454	ARG
1	A	455	LYS
1	A	457	ILE
1	A	461	ASN
1	A	465	TRP
1	A	483	LYS
1	A	485	LYS
1	A	489	SER
1	A	499	THR
1	A	510	LYS
1	A	513	THR
1	A	515	LYS
1	A	518	VAL
1	A	535	CYS
1	A	545	ASN
1	A	558	GLU
1	A	568	LYS
1	A	573	ASP
1	A	574	LYS
1	A	575	LYS
1	A	576	ARG
1	A	582	ASN
1	A	588	SER
1	A	589	LYS
1	A	590	LYS
1	A	591	SER
1	A	592	GLN
1	A	594	ILE
1	A	599	ASN
1	A	621	ASN
1	A	623	THR
1	B	428	GLU
1	B	436	ARG

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Mol	Chain	Res	Type
1	B	437	ASN
1	B	457	ILE
1	B	479	MET
1	B	499	THR
1	B	510	LYS
1	B	530	LEU
1	B	542	ARG
1	B	544	LYS
1	B	558	GLU
1	B	591	SER
1	B	592	GLN
1	B	618	ARG
1	B	621	ASN
1	B	623	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	458	GLN
1	A	461	ASN
1	A	529	HIS
1	A	582	ASN
1	A	585	GLN
1	A	599	ASN
1	A	621	ASN
1	B	491	HIS
1	B	545	ASN
1	B	592	GLN
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 [i](#)

There are no carbohydrates 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	1645	-	5,5,5	0.39	0	5,5,5	0.69	0
2	GOL	A	1646	-	5,5,5	0.36	0	5,5,5	0.60	0
2	GOL	A	1647	-	5,5,5	0.43	0	5,5,5	0.58	0
2	GOL	A	1648	-	5,5,5	0.38	0	5,5,5	0.41	0
2	GOL	A	1649	-	5,5,5	0.26	0	5,5,5	0.59	0
2	GOL	B	1645	-	5,5,5	0.17	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	1645	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1646	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1647	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1648	-	-	0/4/4/4	0/0/0/0
2	GOL	A	1649	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1645	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1645	GOL	2	0
2	A	1648	GOL	1	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](#)

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	227/238 (95%)	0.13	11 (4%) 34 35	31, 57, 91, 99	18 (7%)
1	B	226/238 (94%)	0.39	16 (7%) 19 19	29, 64, 93, 100	13 (5%)
All	All	453/476 (95%)	0.26	27 (5%) 25 25	29, 61, 92, 100	31 (6%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	579	PHE	7.3
1	B	438	GLY	5.7
1	A	576	ARG	5.0
1	B	567	LEU	4.5
1	B	576	ARG	3.7
1	A	572	ILE	3.7
1	B	586	LEU	3.6
1	A	573	ASP	3.5
1	A	504	ALA	3.4
1	B	592	GLN	3.3
1	B	578	GLU	3.3
1	B	585	GLN	3.2
1	B	584	TRP	3.1
1	B	437	ASN	3.0
1	B	582	ASN	2.9
1	A	557	ASN	2.7
1	A	418	ASP	2.7
1	B	575	LYS	2.5
1	A	437	ASN	2.5
1	A	575	LYS	2.4
1	B	574	LYS	2.4
1	A	516	VAL	2.3
1	B	583	GLY	2.3
1	B	555	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	444	LEU	2.2
1	A	518	VAL	2.1
1	B	625[A]	GLN	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	CO	B	1646	1/1	0.99	0.21	3.61	16,16,16,16	1
2	GOL	A	1649	6/6	0.80	0.27	2.74	85,86,92,93	0
2	GOL	A	1645	6/6	0.84	0.35	2.52	65,68,71,74	0
2	GOL	A	1648	6/6	0.56	0.23	1.27	67,80,81,83	0
2	GOL	A	1646	6/6	0.93	0.19	1.16	69,72,76,81	0
2	GOL	B	1645	6/6	0.85	0.20	-	60,64,65,70	0
2	GOL	A	1647	6/6	0.73	0.27	-	52,72,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.