Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 01:39 am BST

PDB ID	:	2WFT
Title	:	Crystal structure of the human HIP ectodomain
Authors	:	Bishop, B.; Aricescu, A.R.; Harlos, K.; O'Callaghan, C.A.; Jones, E.Y.; Siebold, C.
Deposited on	:	2009-04-15
Resolution	:	2.80 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 (i)) were used in the production of this report:

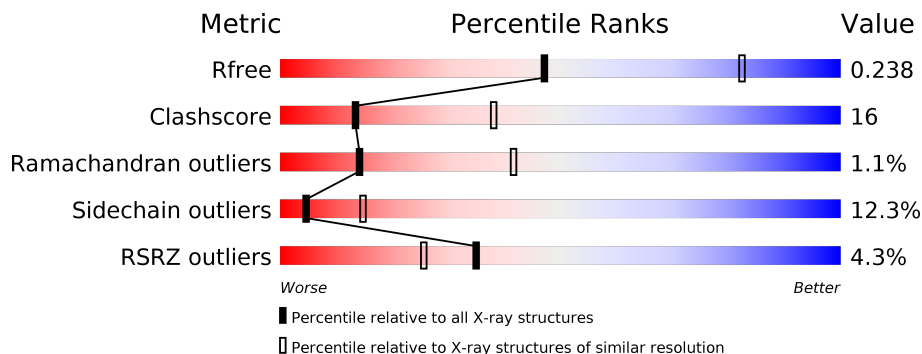|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.80 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	Percentile Ranks	Value
Rfree		0.238
Clashscore		16
Ramachandran outliers		1.1%
Sidechain outliers		12.3%
RSRZ outliers		4.3%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	458	5% / 66% / 24% / 5% ·
1	B	458	3% / 59% / 24% / 5% · / 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6624 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 HEDGEHOG-INTERACTING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total 3414	C 2141	N 605	O 640	S 28	0	0	0
1	B	409	Total 3166	C 1986	N 560	O 592	S 28	0	0	1

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Na 1	0	0
2	A	2	Total 2	Na 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Cl 2	0	0
3	A	1	Total 1	Cl 1	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total 19	O 19	0	0
4	B	19	Total 19	O 19	0	0

3 Residue-property plots ⓘ

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: HEDGEHOG-INTERACTING PROTEIN
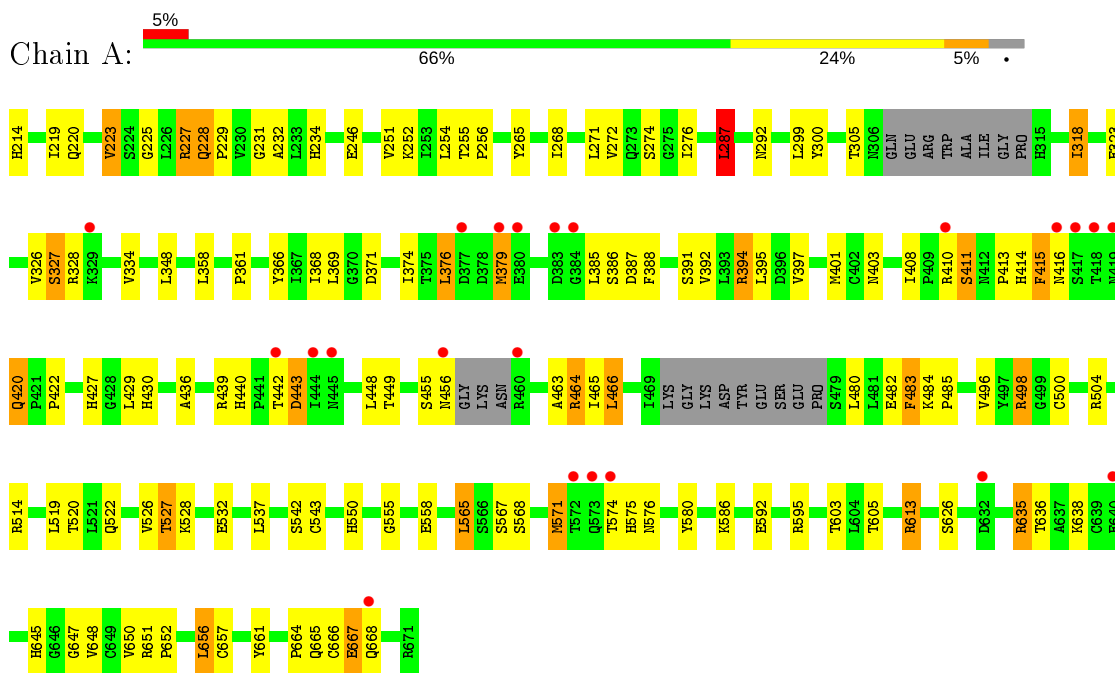
- Molecule 1: HEDGEHOG-INTERACTING PROTEIN
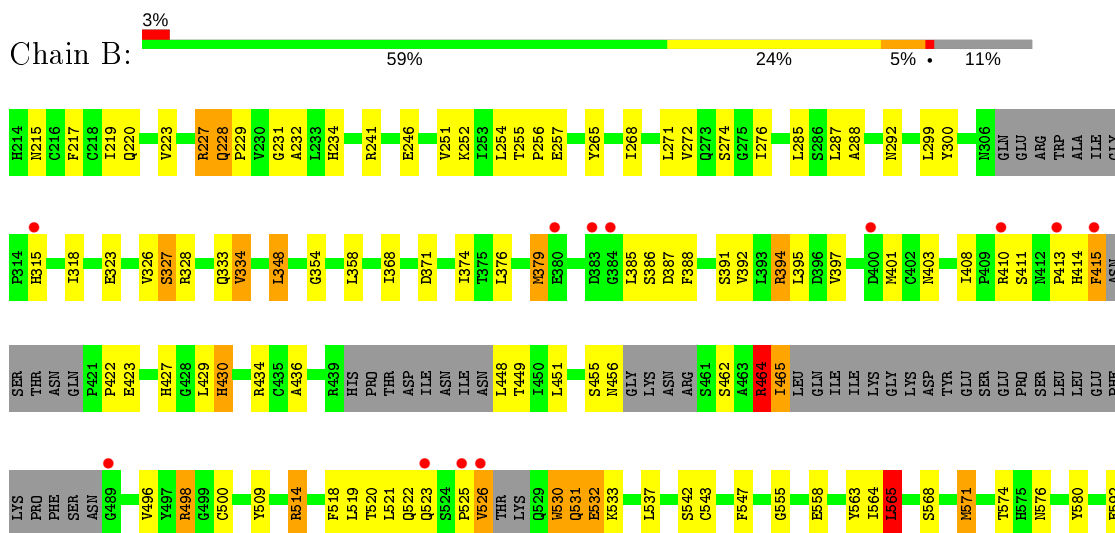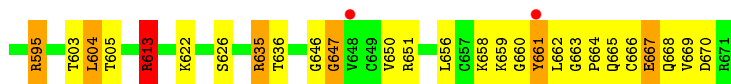
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	100.98Å 100.98Å 305.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.89 – 2.80 19.89 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.89-2.80) 99.7 (19.89-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.10 (at 2.71Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.199 , 0.238 0.198 , 0.238	Depositor DCC
R_{free} test set	2289 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å^2)	67.0	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 66.5	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6624	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	0.63	0/3490	1.08	21/4714 (0.4%)
1	B	0.68	0/3234	1.09	26/4362 (0.6%)
All	All	0.66	0/6724	1.08	47/9076 (0.5%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	613	ARG	NE-CZ-NH2	-14.19	113.20	120.30
1	A	635	ARG	NE-CZ-NH1	13.92	127.26	120.30
1	A	635	ARG	NE-CZ-NH2	-13.45	113.58	120.30
1	B	595	ARG	NE-CZ-NH1	-13.34	113.63	120.30
1	A	498	ARG	NE-CZ-NH2	-13.17	113.71	120.30
1	B	635	ARG	NE-CZ-NH1	-13.14	113.73	120.30
1	A	595	ARG	NE-CZ-NH2	-13.07	113.76	120.30
1	B	394	ARG	NE-CZ-NH2	-13.05	113.78	120.30
1	B	613	ARG	NE-CZ-NH1	-12.66	113.97	120.30
1	A	394	ARG	NE-CZ-NH1	-12.61	114.00	120.30
1	A	613	ARG	NE-CZ-NH1	12.55	126.58	120.30
1	A	328	ARG	NE-CZ-NH2	-12.45	114.07	120.30
1	B	635	ARG	NE-CZ-NH2	12.40	126.50	120.30
1	A	498	ARG	NE-CZ-NH1	12.37	126.48	120.30
1	B	227	ARG	NE-CZ-NH2	-12.28	114.16	120.30
1	A	328	ARG	NE-CZ-NH1	12.15	126.38	120.30
1	B	595	ARG	NE-CZ-NH2	12.11	126.36	120.30
1	B	328	ARG	NE-CZ-NH2	12.02	126.31	120.30
1	B	394	ARG	NE-CZ-NH1	11.90	126.25	120.30
1	A	394	ARG	NE-CZ-NH2	11.71	126.16	120.30
1	B	498	ARG	NE-CZ-NH1	-11.63	114.49	120.30
1	A	227	ARG	NE-CZ-NH2	11.59	126.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	595	ARG	NE-CZ-NH1	11.43	126.01	120.30
1	B	613	ARG	NE-CZ-NH2	11.14	125.87	120.30
1	B	328	ARG	NE-CZ-NH1	-10.90	114.85	120.30
1	A	227	ARG	NE-CZ-NH1	-10.86	114.87	120.30
1	B	227	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	B	498	ARG	NE-CZ-NH2	9.45	125.03	120.30
1	B	635	ARG	CD-NE-CZ	7.27	133.78	123.60
1	A	635	ARG	CD-NE-CZ	6.84	133.18	123.60
1	B	328	ARG	CD-NE-CZ	6.66	132.92	123.60
1	A	613	ARG	CD-NE-CZ	6.65	132.91	123.60
1	A	498	ARG	CD-NE-CZ	6.58	132.81	123.60
1	A	328	ARG	CD-NE-CZ	6.52	132.72	123.60
1	B	595	ARG	CD-NE-CZ	6.29	132.41	123.60
1	B	613	ARG	CD-NE-CZ	6.25	132.34	123.60
1	A	394	ARG	CD-NE-CZ	6.22	132.30	123.60
1	A	595	ARG	CD-NE-CZ	6.16	132.22	123.60
1	A	287	LEU	CA-CB-CG	6.15	129.44	115.30
1	B	227	ARG	CD-NE-CZ	5.79	131.70	123.60
1	B	394	ARG	CD-NE-CZ	5.41	131.17	123.60
1	B	514	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	498	ARG	CD-NE-CZ	5.35	131.09	123.60
1	B	241	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	662	LEU	CA-CB-CG	5.20	127.25	115.30
1	B	662	LEU	CB-CG-CD1	5.09	119.66	111.00
1	B	565	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3414	0	3319	107	1
1	B	3166	0	3071	103	1
2	A	2	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	1	0
3	B	2	0	0	0	0
4	A	19	0	0	2	0
4	B	19	0	0	1	0
All	All	6624	0	6390	209	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 16.

All (209) 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:568:SER:H	1:A:571:MET:CB	1.81	0.94
1:B:659:LYS:O	1:B:661:TYR:HE2	1.51	0.93
1:B:660:GLY:C	1:B:661:TYR:CD2	2.42	0.93
1:A:410:ARG:HA	1:A:415:PHE:HD2	1.35	0.91
1:A:483:PHE:H	1:A:483:PHE:HD2	1.19	0.90
1:B:410:ARG:HA	1:B:415:PHE:HD2	1.36	0.89
1:B:532:GLU:O	1:B:533:LYS:HG3	1.72	0.89
1:B:410:ARG:HA	1:B:415:PHE:CD2	2.09	0.87
1:A:410:ARG:HA	1:A:415:PHE:CD2	2.09	0.86
1:A:645:HIS:CG	1:A:661:TYR:CD1	2.64	0.85
1:A:568:SER:H	1:A:571:MET:HB2	1.42	0.85
1:B:659:LYS:O	1:B:661:TYR:CE2	2.33	0.82
1:B:348:LEU:HD22	1:B:374:ILE:HD12	1.64	0.79
1:A:568:SER:OG	1:A:571:MET:HB2	1.85	0.76
1:A:231:GLY:HA2	1:A:565:LEU:HD13	1.67	0.75
1:A:219:ILE:HD13	1:A:537:LEU:HD13	1.68	0.74
1:B:568:SER:H	1:B:571:MET:CB	2.01	0.74
1:B:650:VAL:HG12	1:B:651:ARG:HG3	1.68	0.74
1:A:568:SER:N	1:A:571:MET:HB2	2.02	0.73
1:A:568:SER:H	1:A:571:MET:HB3	1.52	0.73
1:A:645:HIS:ND1	1:A:661:TYR:CD1	2.56	0.73
1:B:613:ARG:NE	1:B:613:ARG:HA	2.04	0.73
1:B:532:GLU:C	1:B:533:LYS:HG3	2.10	0.72
1:B:568:SER:OG	1:B:571:MET:HB2	1.90	0.70
1:B:660:GLY:C	1:B:661:TYR:CG	2.65	0.70
1:A:440:HIS:HA	3:A:1674:CL:CL	2.28	0.69
1:A:645:HIS:CD2	1:A:661:TYR:CE1	2.80	0.69
1:A:571:MET:HG3	1:A:576:ASN:O	1.93	0.69
1:B:386:SER:O	1:B:387:ASP:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ILE:CD1	1:A:537:LEU:HD13	2.24	0.68
1:B:660:GLY:CA	1:B:661:TYR:CD2	2.77	0.68
1:A:645:HIS:CG	1:A:661:TYR:CE1	2.82	0.68
1:B:658:LYS:O	1:B:661:TYR:HD2	1.77	0.68
1:B:408:ILE:HD12	1:B:422:PRO:HB2	1.75	0.67
1:A:465:ILE:O	1:A:466:LEU:HG	1.94	0.67
1:B:451:LEU:HD13	1:B:509:TYR:CE2	2.31	0.66
1:A:379:MET:HA	1:A:385:LEU:HD12	1.78	0.66
1:A:386:SER:O	1:A:387:ASP:HB2	1.95	0.66
1:A:386:SER:OG	1:A:388:PHE:HB2	1.96	0.66
1:B:246:GLU:OE2	1:B:252:LYS:HE3	1.96	0.66
1:B:568:SER:H	1:B:571:MET:HB3	1.61	0.66
1:A:408:ILE:HD12	1:A:422:PRO:HB2	1.78	0.65
1:B:379:MET:HA	1:B:385:LEU:HD12	1.78	0.65
1:A:246:GLU:OE2	1:A:252:LYS:HE3	1.97	0.65
1:B:231:GLY:HA2	1:B:565:LEU:HD13	1.79	0.65
1:B:523:GLN:HA	1:B:530:TRP:CD1	2.31	0.65
1:B:661:TYR:N	1:B:661:TYR:CD2	2.64	0.64
1:A:394:ARG:C	1:A:395:LEU:HD23	2.17	0.64
1:B:386:SER:OG	1:B:388:PHE:HB2	1.98	0.64
1:A:665:GLN:O	1:A:666:CYS:HB2	1.97	0.64
1:A:255:THR:HB	1:A:256:PRO:HD2	1.81	0.63
1:B:451:LEU:HD13	1:B:509:TYR:HE2	1.63	0.63
1:B:658:LYS:O	1:B:661:TYR:CD2	2.52	0.62
1:A:394:ARG:HH12	1:A:411:SER:HB2	1.65	0.61
1:A:408:ILE:CD1	1:A:422:PRO:HB2	2.31	0.61
1:A:667:GLU:HG2	1:A:668:GLN:HE21	1.63	0.61
1:A:464:ARG:HE	1:A:482:GLU:HG3	1.67	0.60
1:B:568:SER:H	1:B:571:MET:HB2	1.66	0.60
1:A:571:MET:CG	1:A:576:ASN:O	2.49	0.60
1:A:214:HIS:O	1:A:586:LYS:NZ	2.35	0.60
1:A:483:PHE:N	1:A:483:PHE:CD2	2.66	0.59
1:B:571:MET:HG3	1:B:576:ASN:O	2.03	0.59
1:B:531:GLN:H	1:B:531:GLN:HE21	1.51	0.59
1:B:665:GLN:O	1:B:666:CYS:HB2	2.02	0.58
1:A:300:TYR:CE2	1:A:323:GLU:HG3	2.38	0.58
1:A:463:ALA:O	1:A:464:ARG:HG2	2.04	0.58
1:B:436:ALA:HB1	1:B:496:VAL:HG23	1.85	0.57
1:A:464:ARG:HH21	1:A:482:GLU:HG3	1.69	0.57
1:A:532:GLU:O	1:A:532:GLU:HG3	2.04	0.57
1:B:660:GLY:O	1:B:661:TYR:CG	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:GLY:HA3	1:B:661:TYR:CE2	2.40	0.56
1:A:550:HIS:HB2	4:A:2013:HOH:O	2.05	0.56
1:A:214:HIS:NE2	1:B:595:ARG:HD3	2.21	0.56
1:A:526:VAL:HG12	1:A:527:THR:HG22	1.88	0.56
1:B:430:HIS:CD2	1:B:456:ASN:HB2	2.41	0.56
1:B:408:ILE:CD1	1:B:422:PRO:HB2	2.35	0.56
1:B:219:ILE:HD13	1:B:537:LEU:HD13	1.88	0.56
1:A:480:LEU:HD12	1:A:480:LEU:O	2.05	0.56
1:B:522:GLN:O	1:B:530:TRP:HD1	1.89	0.56
1:A:568:SER:N	1:A:571:MET:CB	2.59	0.55
1:B:660:GLY:N	1:B:661:TYR:CD2	2.74	0.55
1:B:394:ARG:C	1:B:395:LEU:HD23	2.27	0.55
1:B:646:GLY:O	1:B:647:GLY:O	2.25	0.55
1:A:229:PRO:HB2	1:A:565:LEU:HD22	1.89	0.54
1:B:430:HIS:HD2	1:B:456:ASN:HB2	1.72	0.54
1:A:647:GLY:HA2	1:A:656:LEU:O	2.07	0.54
1:B:300:TYR:CE2	1:B:323:GLU:HG3	2.43	0.54
1:A:413:PRO:O	1:A:414:HIS:CD2	2.61	0.54
1:B:255:THR:HB	1:B:256:PRO:HD2	1.90	0.54
1:A:483:PHE:CD1	1:A:485:PRO:HG3	2.43	0.54
1:A:219:ILE:HG23	1:A:580:TYR:HB3	1.90	0.54
1:A:645:HIS:ND1	1:A:661:TYR:HD1	2.05	0.54
1:B:523:GLN:HA	1:B:530:TRP:HD1	1.73	0.53
1:A:436:ALA:HB1	1:A:496:VAL:HG23	1.89	0.53
1:A:480:LEU:HD12	1:A:480:LEU:C	2.28	0.53
1:B:251:VAL:HG21	1:B:287:LEU:CD1	2.38	0.53
1:B:415:PHE:C	1:B:415:PHE:HD1	2.12	0.53
1:B:415:PHE:C	1:B:415:PHE:CD1	2.81	0.53
1:B:348:LEU:HD22	1:B:374:ILE:CD1	2.38	0.53
1:A:271:LEU:HD23	1:A:271:LEU:N	2.24	0.52
1:B:568:SER:N	1:B:571:MET:HB2	2.23	0.52
1:B:613:ARG:HA	1:B:613:ARG:HE	1.73	0.52
1:A:415:PHE:CD1	1:A:415:PHE:C	2.83	0.52
1:B:667:GLU:HG2	1:B:668:GLN:HE21	1.75	0.52
1:A:415:PHE:HD1	1:A:415:PHE:C	2.13	0.52
1:A:567:SER:HA	1:A:571:MET:HG2	1.90	0.52
1:A:265:TYR:O	1:A:334:VAL:HG13	2.11	0.51
1:B:229:PRO:HB2	1:B:565:LEU:HD22	1.91	0.51
1:A:650:VAL:HG12	1:A:651:ARG:HG3	1.91	0.51
1:B:268:ILE:O	1:B:272:VAL:HG13	2.11	0.51
1:A:504:ARG:HG2	4:A:2015:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:GLY:CA	1:B:661:TYR:CE2	2.93	0.51
1:A:395:LEU:N	1:A:395:LEU:HD23	2.25	0.51
1:B:326:VAL:HA	1:B:334:VAL:HA	1.92	0.51
1:B:464:ARG:C	1:B:465:ILE:HG22	2.31	0.50
1:B:521:LEU:HD23	1:B:532:GLU:HB2	1.92	0.50
1:A:326:VAL:HA	1:A:334:VAL:HA	1.94	0.50
1:A:234:HIS:ND1	1:A:558:GLU:HG3	2.27	0.50
1:B:659:LYS:C	1:B:661:TYR:CD2	2.85	0.49
1:A:455:SER:O	1:A:456:ASN:HB2	2.12	0.49
1:A:231:GLY:CA	1:A:565:LEU:HD13	2.40	0.49
1:B:571:MET:CG	1:B:576:ASN:O	2.61	0.49
1:B:265:TYR:O	1:B:334:VAL:HG13	2.13	0.49
1:A:300:TYR:OH	1:A:397:VAL:HG11	2.13	0.49
1:A:368:ILE:HG23	1:A:429:LEU:HD13	1.94	0.48
1:B:451:LEU:HD22	1:B:509:TYR:CD2	2.49	0.48
1:A:268:ILE:O	1:A:272:VAL:HG13	2.13	0.48
1:A:466:LEU:HD21	1:A:480:LEU:HB3	1.95	0.48
1:B:219:ILE:HG23	1:B:580:TYR:HB3	1.94	0.48
1:A:449:THR:HA	1:A:466:LEU:O	2.13	0.48
1:B:547:PHE:HB2	1:B:580:TYR:CE2	2.49	0.48
1:A:305:THR:HG22	1:A:318:ILE:HG22	1.95	0.48
1:A:251:VAL:HG21	1:A:287:LEU:HD23	1.96	0.47
1:B:223:VAL:HG11	1:B:254:LEU:HD13	1.94	0.47
1:A:656:LEU:HD12	1:A:657:CYS:N	2.30	0.47
1:B:234:HIS:ND1	1:B:558:GLU:HG3	2.30	0.47
1:B:271:LEU:N	1:B:271:LEU:HD23	2.29	0.47
1:B:386:SER:HB2	4:B:2009:HOH:O	2.14	0.47
1:B:659:LYS:C	1:B:661:TYR:CE2	2.88	0.47
1:B:523:GLN:CA	1:B:530:TRP:CD1	2.96	0.47
1:B:392:VAL:HG23	1:B:429:LEU:HD11	1.97	0.46
1:A:455:SER:O	1:A:456:ASN:CB	2.63	0.46
1:B:219:ILE:CD1	1:B:537:LEU:HD13	2.46	0.46
1:A:414:HIS:ND1	1:A:420:GLN:HB2	2.30	0.46
1:A:483:PHE:HD1	1:A:485:PRO:HG3	1.81	0.45
1:B:232:ALA:O	1:B:555:GLY:HA2	2.17	0.45
1:A:366:TYR:CE1	1:A:394:ARG:HD3	2.52	0.45
1:A:232:ALA:O	1:A:555:GLY:HA2	2.16	0.45
1:B:519:LEU:C	1:B:519:LEU:HD12	2.37	0.45
1:A:361:PRO:HD3	1:A:448:LEU:HD13	1.99	0.44
1:B:413:PRO:O	1:B:414:HIS:CD2	2.70	0.44
1:A:255:THR:HB	1:A:256:PRO:CD	2.47	0.44

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:SER:HA	1:B:427:HIS:HA	1.99	0.44
1:A:368:ILE:HG23	1:A:429:LEU:CD1	2.47	0.44
1:A:326:VAL:HG22	1:A:327:SER:N	2.33	0.44
1:A:371:ASP:O	1:A:374:ILE:HG12	2.18	0.44
1:A:415:PHE:HD1	1:A:416:ASN:HB2	1.82	0.44
1:A:227:ARG:O	1:A:228:GLN:C	2.55	0.43
1:A:519:LEU:HD12	1:A:519:LEU:C	2.38	0.43
1:A:645:HIS:CE1	1:A:661:TYR:CD1	3.06	0.43
1:B:518:PHE:CZ	1:B:564:ILE:HD11	2.53	0.43
1:B:568:SER:N	1:B:571:MET:CB	2.76	0.43
1:B:664:PRO:HB2	1:B:665:GLN:OE1	2.18	0.43
1:A:376:LEU:HD12	1:A:376:LEU:HA	1.77	0.43
1:B:464:ARG:HG2	1:B:464:ARG:H	1.31	0.43
1:A:348:LEU:HD12	1:A:374:ILE:HD12	2.00	0.43
1:B:217:PHE:O	1:B:537:LEU:HA	2.18	0.43
1:A:251:VAL:HG21	1:A:287:LEU:CD2	2.49	0.43
1:B:371:ASP:O	1:B:374:ILE:HG12	2.18	0.43
1:B:518:PHE:HZ	1:B:564:ILE:HD11	1.84	0.43
1:A:413:PRO:C	1:A:414:HIS:CD2	2.92	0.43
1:B:227:ARG:O	1:B:228:GLN:C	2.57	0.43
1:B:368:ILE:HG23	1:B:429:LEU:HD13	2.01	0.43
1:B:663:GLY:HA3	1:B:667:GLU:OE1	2.18	0.43
1:A:305:THR:CG2	1:A:318:ILE:HG22	2.49	0.43
1:A:439:ARG:O	1:A:440:HIS:C	2.57	0.43
1:A:391:SER:HA	1:A:427:HIS:HA	2.01	0.42
1:B:300:TYR:OH	1:B:397:VAL:HG11	2.19	0.42
1:B:410:ARG:HA	1:B:415:PHE:CE2	2.54	0.42
1:A:413:PRO:O	1:A:414:HIS:CG	2.72	0.42
1:A:527:THR:O	1:A:528:LYS:HB2	2.19	0.42
1:B:229:PRO:HB2	1:B:565:LEU:CD2	2.49	0.42
1:A:410:ARG:HA	1:A:415:PHE:CE2	2.52	0.42
1:A:647:GLY:C	1:A:648:VAL:HG23	2.40	0.42
1:A:667:GLU:HG2	1:A:668:GLN:NE2	2.32	0.42
1:B:604:LEU:HD12	1:B:604:LEU:HA	1.86	0.42
1:A:638:LYS:O	1:A:652:PRO:HA	2.20	0.42
1:B:368:ILE:HG23	1:B:429:LEU:CD1	2.50	0.42
1:B:397:VAL:HG12	1:B:397:VAL:O	2.20	0.42
1:A:220:GLN:OE1	1:A:543:CYS:HB2	2.20	0.41
1:B:522:GLN:C	1:B:530:TRP:HD1	2.23	0.41
1:B:220:GLN:OE1	1:B:543:CYS:HB2	2.20	0.41
1:A:664:PRO:HB2	1:A:665:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:LYS:HB2	1:B:533:LYS:HE2	1.68	0.41
1:A:229:PRO:HB2	1:A:565:LEU:CD2	2.49	0.41
1:B:525:PRO:C	1:B:526:VAL:HG12	2.40	0.41
1:B:287:LEU:HD23	1:B:288:ALA:N	2.35	0.41
1:B:327:SER:HB3	1:B:333:GLN:O	2.20	0.41
1:A:225:GLY:HA2	1:A:575:HIS:O	2.21	0.41
1:B:388:PHE:HE1	1:B:423:GLU:HB2	1.85	0.41
1:A:366:TYR:CZ	1:A:394:ARG:HD3	2.56	0.41
1:A:571:MET:HG2	1:A:576:ASN:O	2.21	0.41
1:B:563:TYR:N	1:B:563:TYR:CD2	2.88	0.41
1:A:386:SER:O	1:A:387:ASP:CB	2.66	0.41
1:A:223:VAL:HG11	1:A:254:LEU:HD13	2.03	0.40
1:A:420:GLN:HB2	1:A:420:GLN:HE21	1.68	0.40
1:A:392:VAL:HG23	1:A:429:LEU:HD11	2.03	0.40
1:B:285:LEU:HD13	1:B:354:GLY:O	2.21	0.40
1:B:646:GLY:O	1:B:647:GLY:C	2.60	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:661:TYR:OH	1:B:257:GLU:OE1[5_665]	2.03	0.17

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	430/458 (94%)	397 (92%)	30 (7%)	3 (1%)	22	53
1	B	395/458 (86%)	360 (91%)	29 (7%)	6 (2%)	10	33
All	All	825/916 (90%)	757 (92%)	59 (7%)	9 (1%)	14	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	464	ARG
1	A	274	SER
1	B	647	GLY
1	B	670	ASP
1	B	274	SER
1	A	443	ASP
1	B	215	ASN
1	A	626	SER
1	B	626	SER

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	382/399 (96%)	340 (89%)	42 (11%)	6	19
1	B	352/399 (88%)	304 (86%)	48 (14%)	3	11
All	All	734/798 (92%)	644 (88%)	90 (12%)	4	15

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	VAL
1	A	228	GLN
1	A	276	ILE
1	A	287	LEU
1	A	292	ASN
1	A	299	LEU
1	A	318	ILE
1	A	327	SER
1	A	358	LEU
1	A	369	LEU
1	A	376	LEU
1	A	379	MET
1	A	401	MET
1	A	403	ASN

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Mol	Chain	Res	Type
1	A	411	SER
1	A	415	PHE
1	A	420	GLN
1	A	430	HIS
1	A	442	THR
1	A	443	ASP
1	A	464	ARG
1	A	466	LEU
1	A	483	PHE
1	A	484	LYS
1	A	498	ARG
1	A	500	CYS
1	A	514	ARG
1	A	520	THR
1	A	522	GLN
1	A	527	THR
1	A	542	SER
1	A	565	LEU
1	A	571	MET
1	A	574	THR
1	A	592	GLU
1	A	603	THR
1	A	605	THR
1	A	613	ARG
1	A	635	ARG
1	A	636	THR
1	A	656	LEU
1	A	667	GLU
1	B	228	GLN
1	B	276	ILE
1	B	292	ASN
1	B	299	LEU
1	B	315	HIS
1	B	318	ILE
1	B	327	SER
1	B	334	VAL
1	B	348	LEU
1	B	358	LEU
1	B	376	LEU
1	B	379	MET
1	B	401	MET
1	B	403	ASN

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Mol	Chain	Res	Type
1	B	411	SER
1	B	415	PHE
1	B	430	HIS
1	B	434	ARG
1	B	448	LEU
1	B	449	THR
1	B	455	SER
1	B	462	SER
1	B	464	ARG
1	B	465	ILE
1	B	498	ARG
1	B	500	CYS
1	B	514	ARG
1	B	520	THR
1	B	526	VAL
1	B	530	TRP
1	B	531	GLN
1	B	532	GLU
1	B	542	SER
1	B	565	LEU
1	B	571	MET
1	B	574	THR
1	B	592	GLU
1	B	603	THR
1	B	604	LEU
1	B	605	THR
1	B	613	ARG
1	B	622	LYS
1	B	635	ARG
1	B	636	THR
1	B	656	LEU
1	B	661	TYR
1	B	667	GLU
1	B	669	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	ASN
1	A	414	HIS
1	A	420	GLN
1	A	430	HIS

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Mol	Chain	Res	Type
1	A	456	ASN
1	A	529	GLN
1	A	668	GLN
1	B	292	ASN
1	B	414	HIS
1	B	522	GLN
1	B	529	GLN
1	B	531	GLN
1	B	668	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains (i)

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	438/458 (95%)	-0.20	22 (5%)	28	19	39, 74, 137, 196	0
1	B	409/458 (89%)	-0.24	14 (3%)	45	35	36, 74, 134, 174	0
All	All	847/916 (92%)	-0.22	36 (4%)	35	25	36, 74, 137, 196	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	489	GLY	5.1
1	A	418	THR	4.6
1	A	572	THR	4.5
1	B	415	PHE	4.5
1	A	442	THR	4.3
1	A	417	SER	3.9
1	B	383	ASP	3.8
1	A	380	GLU	3.8
1	A	384	GLY	3.6
1	B	413	PRO	3.3
1	A	419	ASN	3.2
1	A	460	ARG	3.1
1	B	661	TYR	3.1
1	A	444	ILE	3.1
1	A	456	ASN	3.0
1	A	640	GLU	2.9
1	B	648	VAL	2.9
1	B	523	GLN	2.8
1	B	525	PRO	2.8
1	A	445	ASN	2.7
1	A	668	GLN	2.6
1	B	410	ARG	2.6
1	B	380	GLU	2.6
1	A	383	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	416	ASN	2.5
1	A	329	LYS	2.4
1	A	379	MET	2.4
1	A	632	ASP	2.3
1	A	377	ASP	2.2
1	B	526	VAL	2.2
1	B	384	GLY	2.2
1	A	573	GLN	2.2
1	B	315	HIS	2.1
1	A	574	THR	2.1
1	A	410	ARG	2.1
1	B	400	ASP	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
3	CL	A	1674	1/1	0.85	0.64	133,133,133,133	0
3	CL	B	1672	1/1	0.86	0.14	113,113,113,113	0
2	NA	A	1673	1/1	0.94	0.28	116,116,116,116	0
2	NA	A	1672	1/1	0.94	0.35	83,83,83,83	0
3	CL	B	1673	1/1	0.94	0.13	105,105,105,105	0
2	NA	B	1671	1/1	0.95	0.21	75,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.