



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:09 AM GMT

PDB ID : 2FUT
Title : Crystal Structure of Heparinase II Complexed with a Disaccharide Product
Authors : Shaya, D.; Cygler, M.
Deposited on : 2006-01-27
Resolution : 2.30 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

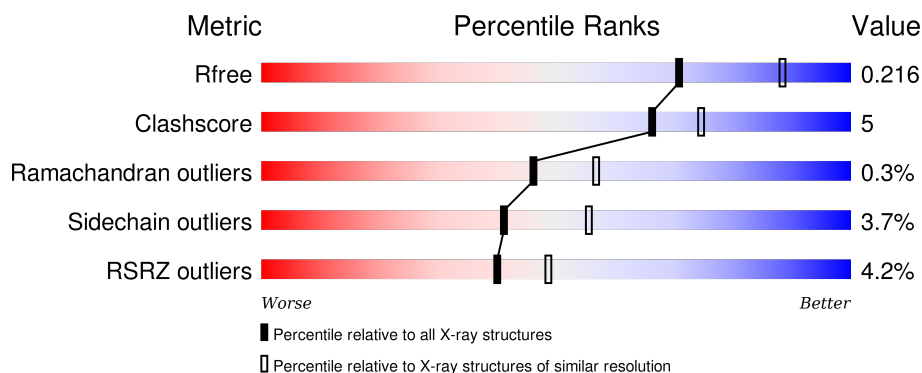
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	748	<div> <div></div> <div>86%12% ..</div> </div>
1	B	748	<div> <div>7%</div> <div>86%12% ..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12752 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 heparinase II protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	743	Total	C	N	O	S	Se	0	0	0
			5949	3832	1003	1091	3	20			
1	B	743	Total	C	N	O	S	Se	0	0	0
			5948	3832	1003	1090	3	20			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	65	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	77	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	80	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	111	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	117	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	154	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	186	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	207	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	209	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	226	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	255	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	275	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	320	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	381	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	396	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	499	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	559	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	603	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	729	MSE	MET	MODIFIED RESIDUE	UNP Q46080
A	758	ALA	PRO	ENGINEERED	UNP Q46080
B	41	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	65	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	77	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	80	MSE	MET	MODIFIED RESIDUE	UNP Q46080

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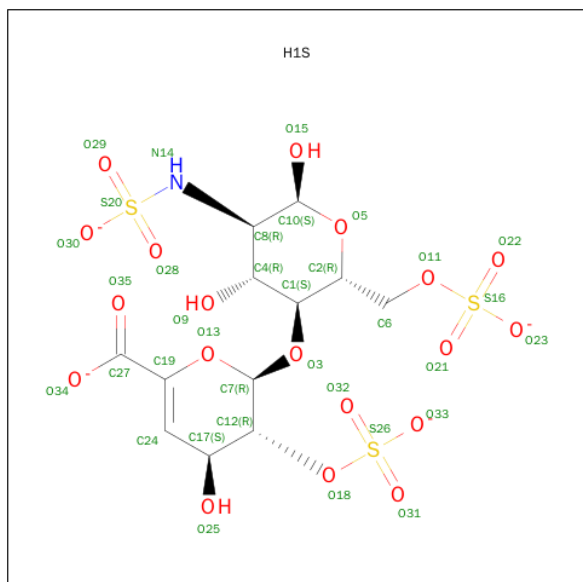
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Chain	Residue	Modelled	Actual	Comment	Reference
B	111	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	117	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	154	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	186	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	207	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	209	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	226	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	255	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	275	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	320	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	381	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	396	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	499	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	559	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	603	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	729	MSE	MET	MODIFIED RESIDUE	UNP Q46080
B	758	ALA	PRO	ENGINEERED	UNP Q46080

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

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

- Molecule 3 is HEPARIN DISACCHARIDE I-S (three-letter code: H1S) (formula: C₁₂H₁₅N O₁₉S₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			35	12	1	19	3		
3	B	1	Total	C	N	O	S	0	0
			35	12	1	19	3		

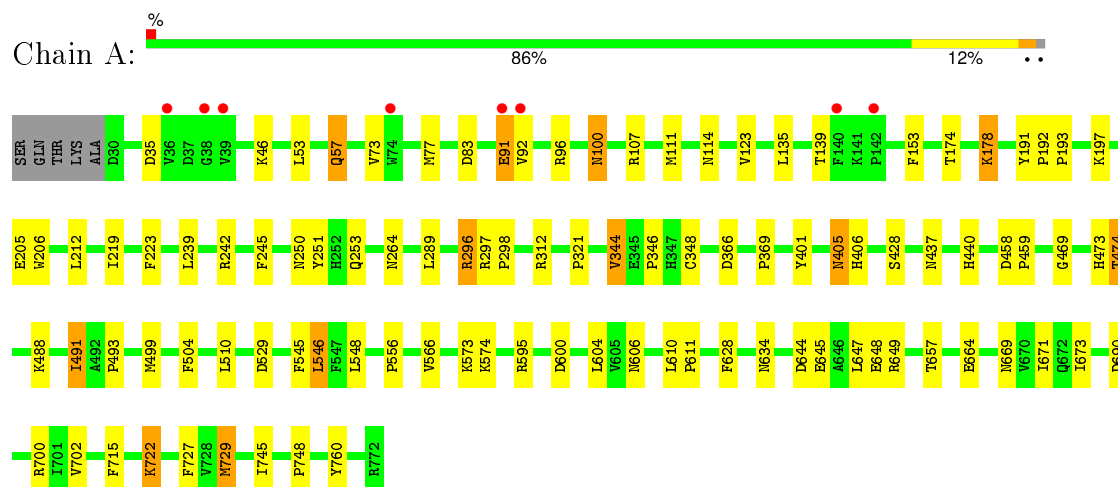
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	547	Total	O	0	0
			547	547		
4	B	236	Total	O	0	0
			236	236		

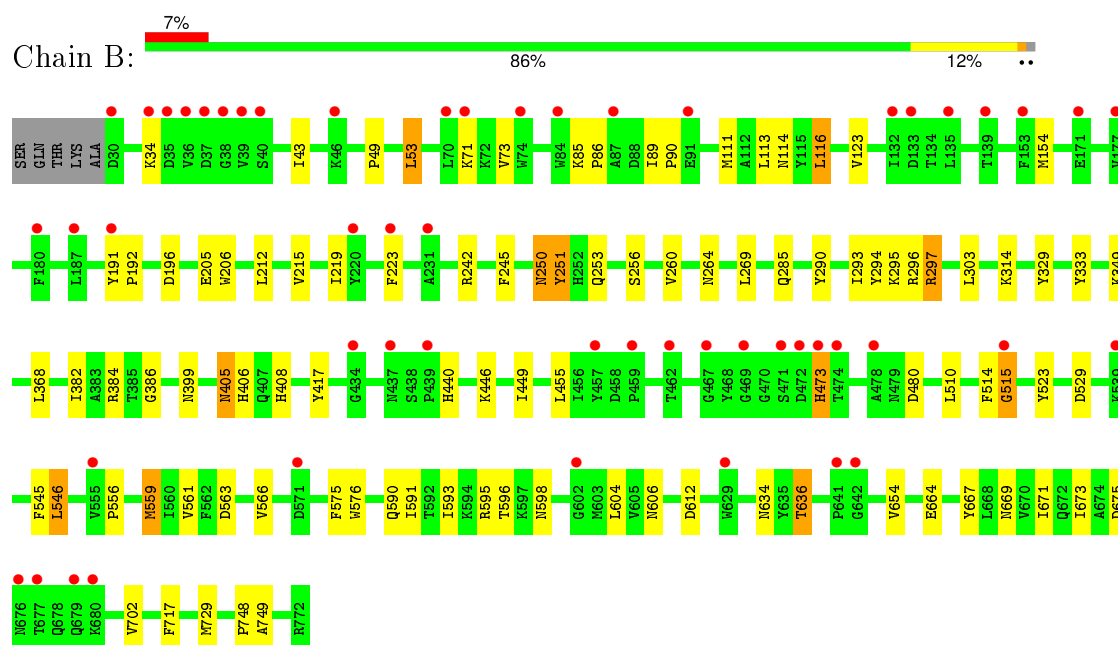
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($RSRZ > 2$). 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: heparinase II protein



- Molecule 1: heparinase II protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.10Å 163.30Å 95.30Å 90.00° 105.50° 90.00°	Depositor
Resolution (Å)	91.67 – 2.30 47.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (91.67-2.30) 96.0 (47.99-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.176 , 0.221 0.176 , 0.216	Depositor DCC
R_{free} test set	3309 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.790	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.8	EDS
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 65137 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12752	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, H1S

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	0.46	0/6091	0.59	0/8212
1	B	0.39	0/6090	0.53	0/8210
All	All	0.42	0/12181	0.56	0/16422

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	91	GLU	Peptide

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	5949	0	5859	62	0
1	B	5948	0	5859	59	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	35	0	15	1	0
3	B	35	0	15	0	0
4	A	547	0	0	6	0
4	B	236	0	0	1	0
All	All	12752	0	11748	117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (117) 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:296:ARG:HH11	1:A:296:ARG:HG2	1.30	0.96
1:B:717:PHE:HE1	1:B:729:MSE:HE1	1.29	0.95
1:B:606:ASN:HD21	1:B:669:ASN:HB3	1.29	0.94
1:B:473:HIS:H	1:B:473:HIS:CD2	1.85	0.94
1:B:717:PHE:CE1	1:B:729:MSE:HE1	2.04	0.93
1:B:473:HIS:H	1:B:473:HIS:HD2	1.22	0.86
1:A:53:LEU:HB2	1:A:57:GLN:HG3	1.67	0.76
1:A:253:GLN:HE22	1:A:406:HIS:H	1.33	0.75
1:A:296:ARG:HH11	1:A:296:ARG:CG	1.99	0.74
1:A:574:LYS:O	1:A:657:THR:HG23	1.88	0.73
1:B:253:GLN:HE22	1:B:406:HIS:H	1.37	0.73
1:B:559:MSE:CE	1:B:561:VAL:HG22	2.21	0.70
1:A:573:LYS:HE2	1:A:657:THR:HG21	1.72	0.70
1:A:428:SER:H	1:A:440:HIS:HE1	1.39	0.70
1:B:253:GLN:HE22	1:B:405:ASN:HB3	1.57	0.68
1:A:606:ASN:HD21	1:A:669:ASN:HB3	1.60	0.66
1:B:114:ASN:HD22	1:B:123:VAL:HG11	1.61	0.65
1:A:628:PHE:H	1:A:634:ASN:HD21	1.45	0.65
1:B:514:PHE:O	1:B:515:GLY:O	2.15	0.64
1:A:297:ARG:NH2	1:A:648:GLU:OE1	2.31	0.64
1:B:556:PRO:HD2	1:B:673:ILE:O	1.98	0.64
1:A:96:ARG:HD2	4:A:1264:HOH:O	1.98	0.64
1:B:455:LEU:HB2	1:B:575:PHE:HB2	1.81	0.62
1:A:573:LYS:CE	1:A:657:THR:HG21	2.30	0.62
1:A:114:ASN:HD22	1:A:123:VAL:HG11	1.65	0.62
1:B:205:GLU:HG2	1:B:260:VAL:HG22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:MSE:HE2	1:B:561:VAL:HG22	1.81	0.60
1:B:473:HIS:N	1:B:473:HIS:CD2	2.63	0.60
1:A:474:THR:HG21	4:A:1000:HOH:O	2.01	0.60
1:A:253:GLN:HE22	1:A:405:ASN:HB3	1.65	0.60
1:B:595:ARG:HH12	1:B:598:ASN:HD22	1.49	0.59
1:B:559:MSE:HE1	1:B:561:VAL:HG22	1.85	0.59
1:A:428:SER:H	1:A:440:HIS:CE1	2.20	0.58
1:B:250:ASN:HD22	1:B:251:TYR:H	1.51	0.58
1:A:566:VAL:HG22	1:A:664:GLU:HG3	1.84	0.58
1:A:760:TYR:HE1	4:A:910:HOH:O	1.87	0.57
1:B:546:LEU:HD22	1:B:702:VAL:HG21	1.87	0.57
1:A:748:PRO:HB2	1:B:368:LEU:HD23	1.86	0.56
1:A:197:LYS:HE3	1:A:491:ILE:HD12	1.88	0.56
1:B:515:GLY:HA2	1:B:523:TYR:CD2	2.41	0.56
1:A:289:LEU:HD21	1:A:321:PRO:HB2	1.88	0.56
1:A:297:ARG:HB3	1:A:298:PRO:HD2	1.88	0.55
1:A:297:ARG:HH22	1:A:648:GLU:CD	2.10	0.55
1:B:294:TYR:HB3	1:B:382:ILE:HG12	1.88	0.55
1:B:545:PHE:HD2	1:B:559:MSE:HE1	1.73	0.53
1:A:469:GLY:O	1:A:473:HIS:HE1	1.91	0.53
1:A:644:ASP:OD2	1:A:649:ARG:HD2	2.08	0.53
1:B:296:ARG:O	1:B:384:ARG:NH2	2.43	0.52
1:B:111:MSE:HE3	1:B:123:VAL:HG13	1.91	0.52
1:A:253:GLN:NE2	1:A:406:HIS:H	2.06	0.52
1:A:510:LEU:HD11	1:A:529:ASP:HB2	1.92	0.52
1:B:634:ASN:ND2	1:B:636:THR:HG23	2.26	0.51
1:A:546:LEU:HD22	1:A:702:VAL:HG21	1.93	0.51
1:B:253:GLN:NE2	1:B:406:HIS:H	2.07	0.51
1:A:722:LYS:N	1:A:722:LYS:HD2	2.26	0.50
1:A:206:TRP:HA	1:A:264:ASN:OD1	2.12	0.49
1:B:219:ILE:HD12	1:B:223:PHE:HB3	1.94	0.49
1:B:269:LEU:HD13	1:B:285:GLN:HE22	1.78	0.48
1:B:606:ASN:HD22	1:B:671:ILE:HG13	1.78	0.48
1:A:83:ASP:OD1	1:A:107:ARG:NH2	2.47	0.47
1:A:111:MSE:HG2	4:A:1269:HOH:O	2.14	0.47
1:A:344:VAL:HG13	1:A:348:CYS:HB2	1.95	0.47
1:A:219:ILE:HD12	1:A:223:PHE:HB3	1.96	0.47
1:A:191:TYR:HA	1:A:192:PRO:C	2.36	0.47
1:A:745:ILE:HD13	1:B:333:TYR:HE1	1.79	0.47
1:B:53:LEU:HD11	1:B:116:LEU:HD11	1.97	0.46
1:B:49:PRO:HG3	1:B:116:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:ILE:HD12	1:B:604:LEU:HD22	1.97	0.45
1:B:285:GLN:NE2	1:B:329:TYR:OH	2.47	0.45
1:B:154:MSE:HE2	1:B:215:VAL:HG21	1.99	0.45
1:A:107:ARG:HD2	4:A:1216:HOH:O	2.17	0.45
1:A:437:ASN:ND2	1:A:469:GLY:HA3	2.32	0.44
1:B:515:GLY:HA2	1:B:523:TYR:CE2	2.51	0.44
1:B:510:LEU:HD11	1:B:529:ASP:HB2	1.99	0.44
1:B:191:TYR:HA	1:B:192:PRO:C	2.37	0.44
1:B:748:PRO:HD2	4:B:806:HOH:O	2.18	0.44
1:A:645:GLU:HB3	4:A:1234:HOH:O	2.17	0.44
1:A:178:LYS:N	1:A:178:LYS:HD3	2.32	0.44
1:A:312:ARG:HH22	1:A:600:ASP:CG	2.20	0.43
1:A:556:PRO:HD2	1:A:673:ILE:O	2.19	0.43
1:B:297:ARG:HD3	1:B:417:TYR:CE1	2.53	0.43
1:A:100:ASN:HD22	1:A:346:PRO:HG2	1.83	0.43
1:A:73:VAL:O	1:A:77:MSE:HG3	2.19	0.43
1:B:242:ARG:HA	1:B:245:PHE:CE2	2.53	0.43
1:B:206:TRP:HA	1:B:264:ASN:OD1	2.19	0.43
1:B:34:LYS:HB2	1:B:43:ILE:HD11	2.01	0.43
1:B:576:TRP:HB2	1:B:667:TYR:CE2	2.54	0.43
1:A:690:ASP:O	1:A:715:PHE:HB2	2.19	0.43
1:B:566:VAL:HG22	1:B:664:GLU:HG3	2.00	0.43
1:A:604:LEU:HG	1:A:671:ILE:HG23	2.01	0.42
1:A:727:PHE:HB3	1:A:729:MSE:HE3	2.01	0.42
1:A:174:THR:HG23	1:A:178:LYS:HE2	2.02	0.42
1:A:296:ARG:NH1	1:A:296:ARG:HG2	2.09	0.42
1:A:745:ILE:HD13	1:B:333:TYR:CE1	2.54	0.42
1:B:606:ASN:ND2	1:B:669:ASN:HB3	2.14	0.42
1:B:73:VAL:HG23	1:B:349:LYS:HD2	2.01	0.42
1:B:591:ILE:HD13	1:B:654:VAL:HG11	2.02	0.42
1:B:290:TYR:HA	1:B:293:ILE:HD12	2.02	0.42
1:B:85:LYS:HA	1:B:86:PRO:HD3	1.93	0.42
1:A:192:PRO:HA	1:A:193:PRO:HD3	1.86	0.41
1:A:53:LEU:HB2	1:A:57:GLN:CG	2.43	0.41
1:B:384:ARG:NH1	1:B:386:GLY:O	2.51	0.41
1:A:135:LEU:HA	1:A:153:PHE:CE2	2.56	0.41
1:A:401:TYR:HB3	1:A:499:MSE:HE2	2.01	0.41
1:A:458:ASP:HA	1:A:459:PRO:HD2	1.95	0.41
1:B:563:ASP:HB2	1:B:667:TYR:HB2	2.02	0.41
1:A:493:PRO:HD3	1:A:504:PHE:CE2	2.56	0.41
1:B:449:ILE:HB	1:B:480:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:HIS:CD2	1:B:446:LYS:HG2	2.56	0.41
1:A:57:GLN:HE21	1:A:57:GLN:HB3	1.59	0.41
1:A:205:GLU:OE2	3:A:801:H1S:O35	2.39	0.41
1:A:242:ARG:HA	1:A:245:PHE:CE2	2.56	0.41
1:B:89:ILE:HA	1:B:90:PRO:HD3	1.97	0.41
1:A:369:PRO:HG2	1:B:749:ALA:HB3	2.03	0.41
1:A:548:LEU:HD22	1:A:700:ARG:HH11	1.86	0.40
1:B:408:HIS:CD2	1:B:446:LYS:HA	2.56	0.40
1:A:610:LEU:HA	1:A:611:PRO:C	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	741/748 (99%)	711 (96%)	29 (4%)	1 (0%)	56	68
1	B	741/748 (99%)	699 (94%)	39 (5%)	3 (0%)	39	48
All	All	1482/1496 (99%)	1410 (95%)	68 (5%)	4 (0%)	46	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	515	GLY
1	B	440	HIS
1	A	91	GLU
1	B	399	ASN

5.3.2 Protein sidechains ⓘ

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	630/614 (103%)	606 (96%)	24 (4%)	40	54
1	B	630/614 (103%)	608 (96%)	22 (4%)	43	58
All	All	1260/1228 (103%)	1214 (96%)	46 (4%)	41	55

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

Mol	Chain	Res	Type
1	A	35	ASP
1	A	46	LYS
1	A	57	GLN
1	A	92	VAL
1	A	100	ASN
1	A	139	THR
1	A	178	LYS
1	A	212	LEU
1	A	239	LEU
1	A	250	ASN
1	A	251	TYR
1	A	296	ARG
1	A	344	VAL
1	A	366	ASP
1	A	405	ASN
1	A	474	THR
1	A	488	LYS
1	A	491	ILE
1	A	545	PHE
1	A	546	LEU
1	A	595	ARG
1	A	647	LEU
1	A	722	LYS
1	A	729	MSE
1	B	53	LEU
1	B	71	LYS
1	B	113	LEU

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Mol	Chain	Res	Type
1	B	116	LEU
1	B	196	ASP
1	B	212	LEU
1	B	250	ASN
1	B	251	TYR
1	B	256	SER
1	B	295	LYS
1	B	297	ARG
1	B	303	LEU
1	B	314	LYS
1	B	405	ASN
1	B	473	HIS
1	B	546	LEU
1	B	559	MSE
1	B	590	GLN
1	B	596	THR
1	B	612	ASP
1	B	636	THR
1	B	675	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	100	ASN
1	A	114	ASN
1	A	253	GLN
1	A	285	GLN
1	A	437	ASN
1	A	440	HIS
1	A	473	HIS
1	A	606	ASN
1	A	634	ASN
1	A	669	ASN
1	A	738	GLN
1	B	114	ASN
1	B	228	ASN
1	B	250	ASN
1	B	253	GLN
1	B	285	GLN
1	B	473	HIS
1	B	583	GLN

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Mol	Chain	Res	Type
1	B	598	ASN
1	B	606	ASN
1	B	669	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
3	H1S	A	801	-	31,36,36	1.82	5 (16%)	35,56,56	1.08	2 (5%)
3	H1S	B	802	-	31,36,36	1.96	4 (12%)	35,56,56	1.30	4 (11%)

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
3	H1S	A	801	-	-	0/20/60/60	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H1S	B	802	-	-	0/20/60/60	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	H1S	O18-S26	2.26	1.64	1.57
3	A	801	H1S	O11-S16	2.31	1.64	1.57
3	B	802	H1S	O18-S26	2.33	1.64	1.57
3	A	801	H1S	O13-C19	4.05	1.45	1.37
3	B	802	H1S	O13-C19	4.31	1.46	1.37
3	A	801	H1S	O29-S20	5.18	1.47	1.42
3	A	801	H1S	O28-S20	5.89	1.48	1.42
3	B	802	H1S	O28-S20	5.92	1.48	1.42
3	B	802	H1S	O29-S20	6.16	1.48	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	H1S	O13-C19-C24	-3.98	118.34	124.12
3	B	802	H1S	C4-C8-N14	-2.55	105.58	110.64
3	A	801	H1S	O13-C19-C24	-2.54	120.43	124.12
3	B	802	H1S	C6-C2-C1	-2.32	107.47	113.35
3	B	802	H1S	C17-C24-C19	-2.05	118.13	121.60
3	A	801	H1S	O28-S20-N14	2.29	111.56	108.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	H1S	1	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	723/748 (96%)	-0.05	8 (1%) 82 86	2, 10, 25, 44	0
1	B	723/748 (96%)	0.53	53 (7%) 18 25	9, 28, 45, 54	0
All	All	1446/1496 (96%)	0.24	61 (4%) 40 49	2, 18, 40, 54	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	38	GLY	7.5
1	A	39	VAL	4.7
1	B	71	LYS	4.6
1	B	473	HIS	4.6
1	B	39	VAL	4.3
1	A	38	GLY	4.0
1	B	37	ASP	3.9
1	B	139	THR	3.7
1	B	478	ALA	3.4
1	B	133	ASP	3.4
1	B	515	GLY	3.3
1	B	680	LYS	3.1
1	A	36	VAL	3.0
1	B	191	TYR	3.0
1	A	91	GLU	3.0
1	B	135	LEU	3.0
1	B	539	LYS	2.9
1	B	74	TRP	2.9
1	B	602	GLY	2.9
1	B	132	ILE	2.9
1	B	153	PHE	2.9
1	B	91	GLU	2.9
1	B	472	ASP	2.9
1	B	439	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	474	THR	2.7
1	B	180	PHE	2.7
1	B	187	LEU	2.7
1	B	437	ASN	2.6
1	B	171	GLU	2.6
1	B	36	VAL	2.6
1	B	35	ASP	2.6
1	B	679	GLN	2.6
1	B	70	LEU	2.6
1	B	30	ASP	2.5
1	B	462	THR	2.5
1	B	467	GLY	2.4
1	B	46	LYS	2.4
1	B	434	GLY	2.4
1	B	177	VAL	2.4
1	B	555	VAL	2.4
1	B	87	ALA	2.4
1	B	223	PHE	2.4
1	B	571	ASP	2.4
1	B	642	GLY	2.3
1	B	677	THR	2.2
1	B	471	SER	2.2
1	B	629	TRP	2.2
1	A	74	TRP	2.2
1	B	220	TYR	2.1
1	B	469	GLY	2.1
1	B	641	PRO	2.1
1	B	34	LYS	2.1
1	B	40	SER	2.1
1	B	84	TRP	2.1
1	B	457	TYR	2.1
1	B	676	ASN	2.1
1	A	142	PRO	2.1
1	B	459	PRO	2.1
1	A	92	VAL	2.1
1	B	231	ALA	2.0
1	A	140	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
3	H1S	B	802	35/35	0.88	0.19	0.18	46,50,58,58	0
3	H1S	A	801	35/35	0.96	0.12	-0.43	14,17,30,31	0
2	ZN	A	1	1/1	0.99	0.02	-4.70	10,10,10,10	0
2	ZN	B	2	1/1	0.98	0.03	-6.57	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.