



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:37 PM UTC

PDB ID : 3S96 / pdb_00003s96
Title : Crystal structure of 3B5H10
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Deposited on : 2011-05-31
Resolution : 1.90 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
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

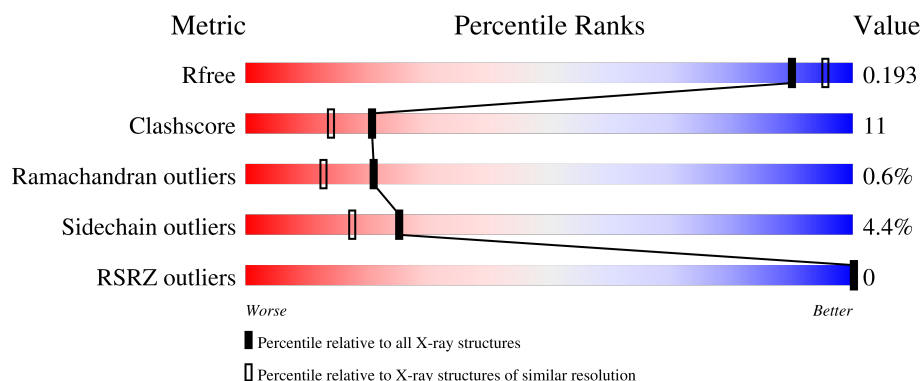
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	220	 80% 19% ..
1	C	220	 82% 14% ...
2	B	218	 73% 19% • 6%
2	D	218	 75% 15% •• 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7310 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 3B5H10 FAB heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1660	1067	265	321	7			
1	C	218	Total	C	N	O	S	0	0	0
			1659	1067	265	320	7			

- Molecule 2 is a protein called 3B5H10 FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total	C	N	O	S	0	0	0
			1555	980	256	313	6			
2	D	203	Total	C	N	O	S	1	0	0
			1546	975	254	311	6			

- Molecule 3 is water.

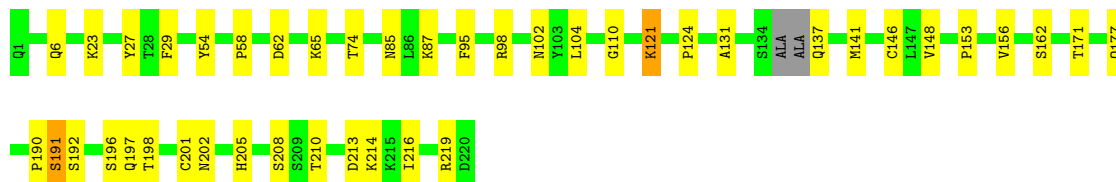
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	228	Total	O	0	0
			228	228		
3	B	213	Total	O	0	0
			213	213		
3	C	217	Total	O	0	0
			217	217		
3	D	232	Total	O	0	0
			232	232		

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.

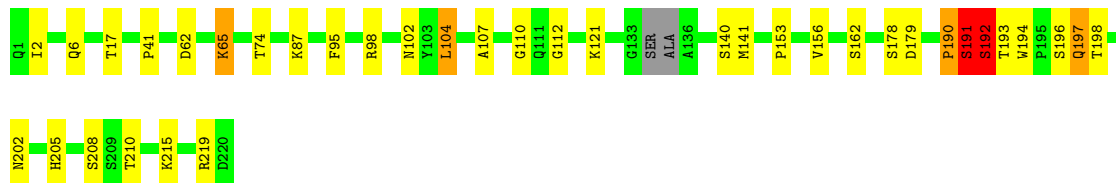
- Molecule 1: 3B5H10 FAB heavy chain

Chain A: 



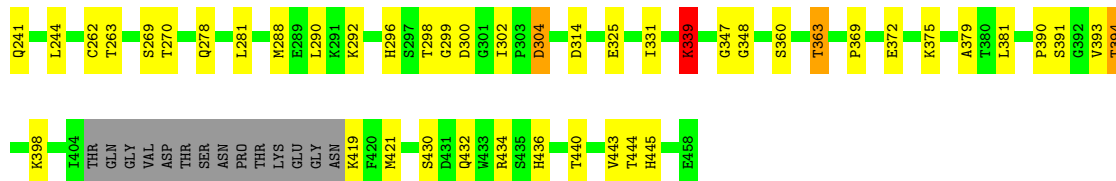
- Molecule 1: 3B5H10 FAB heavy chain

Chain C: 



- Molecule 2: 3B5H10 FAB light chain

Chain B: 



- Molecule 2: 3B5H10 FAB light chain

Chain D: 



LYS	GLU	GLY	ASN	K419	H427	S430	D431	Q432	W433	R434	S435	H436	N437	T440	V443	E451	E458
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.26Å 78.25Å 123.62Å 90.00° 90.23° 90.00°	Depositor
Resolution (Å)	11.00 – 1.90 11.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (11.00-1.90) 87.7 (11.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.25 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.183 , 0.260 0.188 , 0.193	Depositor DCC
R_{free} test set	3005 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.419 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7310	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	2/1709 (0.1%)	1.00	3/2339 (0.1%)
1	C	1.00	0/1708	1.05	3/2338 (0.1%)
2	B	0.97	0/1591	0.98	1/2161 (0.0%)
2	D	1.06	1/1582 (0.1%)	1.02	5/2149 (0.2%)
All	All	1.01	3/6590 (0.0%)	1.01	12/8987 (0.1%)

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	C	0	2
2	D	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	399	ALA	CA-CB	18.12	1.88	1.53
1	A	124	PRO	CA-C	6.00	1.56	1.52
1	A	171	THR	CA-CB	5.09	1.60	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	65	LYS	N-CA-C	11.42	123.29	111.07
2	D	389	SER	N-CA-C	6.49	124.15	109.81
1	A	190	PRO	CA-C-N	-6.31	113.78	122.30
1	A	190	PRO	C-N-CA	-6.31	113.78	122.30
1	C	192	SER	N-CA-C	-5.95	98.14	110.80
2	D	388	PHE	CA-C-N	5.86	136.09	121.80
2	D	388	PHE	C-N-CA	5.86	136.09	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	269	SER	N-CA-C	5.81	119.18	111.75
2	D	388	PHE	N-CA-C	-5.34	102.01	109.69
2	D	365	THR	CB-CA-C	5.12	119.49	109.35
1	A	29	PHE	N-CA-C	5.08	117.21	111.11
1	C	178	SER	N-CA-C	5.04	118.57	111.52

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	190	PRO	Peptide
1	C	191	SER	Peptide
2	D	388	PHE	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	1660	0	1609	33	0
1	C	1659	0	1609	36	0
2	B	1555	0	1511	44	0
2	D	1546	0	1503	27	0
3	A	228	0	0	17	0
3	B	213	0	0	12	1
3	C	217	0	0	12	1
3	D	232	0	0	13	0
All	All	7310	0	6232	140	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 11.

All (140) 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:C:104:LEU:HD11	3:D:659:HOH:O	1.40	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:GLN:HB2	3:B:654:HOH:O	1.46	1.15
2:B:263:THR:HB	3:B:576:HOH:O	1.52	1.07
2:B:372:GLU:O	2:B:375:LYS:HG2	1.56	1.06
1:A:201:CYS:SG	3:A:425:HOH:O	2.20	0.99
1:A:87:LYS:HE3	3:A:243:HOH:O	1.63	0.98
1:A:201:CYS:HB2	3:A:425:HOH:O	1.65	0.96
1:A:146:CYS:SG	3:A:425:HOH:O	2.26	0.94
2:B:288:MET:HE2	2:B:290:LEU:HB2	1.49	0.94
2:B:288:MET:HE3	2:B:296:HIS:HB2	1.51	0.89
1:C:190:PRO:O	1:C:193:THR:HB	1.74	0.87
1:A:62:ASP:HA	1:A:65:LYS:HE2	1.56	0.86
1:A:201:CYS:CB	3:A:425:HOH:O	2.20	0.85
2:B:263:THR:HG22	2:B:314:ASP:OD1	1.77	0.84
1:C:162:SER:H	1:C:202:ASN:HD21	1.25	0.83
2:D:402:THR:HG23	3:D:519:HOH:O	1.79	0.82
2:D:288:MET:HE1	2:D:308:GLY:HA3	1.64	0.78
1:C:74:THR:HG21	3:C:393:HOH:O	1.86	0.75
2:B:363:THR:HG21	3:B:650:HOH:O	1.87	0.75
2:D:340:GLU:OE2	3:D:685:HOH:O	2.05	0.75
1:C:193:THR:HG21	3:C:432:HOH:O	1.86	0.74
2:B:300:ASP:HB2	2:B:302:ILE:HG12	1.69	0.74
2:B:393:VAL:HG21	2:B:443:VAL:HG13	1.71	0.73
2:D:419:LYS:N	3:D:653:HOH:O	2.20	0.73
1:A:153:PRO:O	1:A:205:HIS:HE1	1.72	0.72
1:A:210:THR:HG22	3:A:268:HOH:O	1.90	0.72
2:D:373:GLU:HG2	2:D:378:LYS:HB2	1.70	0.71
2:B:331:ILE:HD12	3:B:654:HOH:O	1.90	0.71
2:B:360:SER:CB	2:B:419:LYS:HZ1	2.04	0.71
2:B:393:VAL:CG2	2:B:443:VAL:HG13	2.21	0.70
2:D:400:ASN:HD21	2:D:437:ASN:H	1.38	0.70
2:D:402:THR:HB	3:D:673:HOH:O	1.92	0.70
2:B:372:GLU:HG2	3:B:653:HOH:O	1.90	0.69
2:B:288:MET:HE3	2:B:296:HIS:CB	2.21	0.68
2:B:292:LYS:HE3	3:B:579:HOH:O	1.96	0.66
2:B:241:GLN:HE22	2:B:347:GLY:HA2	1.62	0.65
2:B:241:GLN:HG2	3:B:563:HOH:O	1.97	0.65
2:B:393:VAL:HG21	2:B:443:VAL:CG1	2.28	0.64
1:C:162:SER:H	1:C:202:ASN:ND2	1.95	0.64
2:B:360:SER:CB	2:B:419:LYS:NZ	2.62	0.63
2:B:244:LEU:HD22	2:B:262:CYS:SG	2.39	0.63
1:C:191:SER:O	1:C:192:SER:OG	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:HIS:HD2	1:A:208:SER:OG	1.82	0.62
2:B:288:MET:CE	2:B:296:HIS:CB	2.78	0.61
1:C:191:SER:C	1:C:192:SER:O	2.37	0.60
2:B:394:THR:HG23	2:B:444:THR:HB	1.83	0.60
1:A:162:SER:H	1:A:202:ASN:HD21	1.50	0.60
2:D:288:MET:HE1	2:D:308:GLY:CA	2.32	0.59
2:D:292:LYS:HE3	2:D:293:ASP:HB3	1.85	0.59
2:D:419:LYS:HG3	3:D:621:HOH:O	2.01	0.59
2:B:299:GLY:HA2	2:B:300:ASP:HB2	1.85	0.58
2:B:360:SER:HB2	2:B:419:LYS:NZ	2.17	0.58
2:B:360:SER:HB2	2:B:419:LYS:HZ1	1.67	0.58
1:A:202:ASN:OD1	1:A:213:ASP:OD1	2.23	0.57
2:B:421:MET:HE3	3:B:645:HOH:O	2.05	0.57
2:D:242:LEU:N	3:D:647:HOH:O	2.38	0.56
1:A:58:PRO:HD2	3:A:421:HOH:O	2.04	0.56
1:C:6:GLN:HE21	1:C:110:GLY:HA3	1.71	0.56
1:C:104:LEU:CD1	3:D:659:HOH:O	2.18	0.56
2:B:375:LYS:HE2	3:B:573:HOH:O	2.04	0.56
1:C:215:LYS:HE3	3:C:434:HOH:O	2.06	0.55
1:C:193:THR:HA	3:C:401:HOH:O	2.06	0.55
1:C:62:ASP:O	1:C:65:LYS:HG2	2.07	0.55
1:C:140:SER:O	1:C:191:SER:CB	2.54	0.55
1:A:54:TYR:HA	3:A:438:HOH:O	2.05	0.54
1:C:198:THR:HB	3:C:434:HOH:O	2.07	0.54
1:A:198:THR:HG22	3:A:399:HOH:O	2.08	0.53
1:C:153:PRO:O	1:C:205:HIS:HE1	1.91	0.53
1:A:6:GLN:HE22	1:A:95:PHE:HA	1.73	0.53
1:A:162:SER:H	1:A:202:ASN:ND2	2.08	0.52
1:A:137:GLN:N	3:A:444:HOH:O	2.41	0.52
2:B:445:HIS:HD2	3:B:623:HOH:O	1.92	0.52
1:C:191:SER:N	1:C:192:SER:O	2.42	0.52
2:B:299:GLY:HA2	2:B:302:ILE:HG12	1.92	0.52
1:A:102:ASN:HB3	3:A:427:HOH:O	2.10	0.52
2:D:398:LYS:HB2	2:D:440:THR:HB	1.92	0.52
1:C:197:GLN:HE21	1:C:197:GLN:HA	1.75	0.51
1:C:179:ASP:OD1	1:C:179:ASP:O	2.29	0.51
2:B:393:VAL:CG2	2:B:443:VAL:CG1	2.89	0.51
1:C:140:SER:O	1:C:191:SER:OG	2.26	0.51
2:D:430:SER:O	2:D:434:ARG:HG3	2.11	0.51
2:B:325:GLU:HG2	3:B:505:HOH:O	2.11	0.50
1:C:6:GLN:HE22	1:C:95:PHE:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:SER:HB3	3:C:262:HOH:O	2.10	0.50
2:B:369:PRO:HD3	2:B:381:LEU:CD2	2.40	0.50
1:A:6:GLN:HE21	1:A:110:GLY:HA3	1.76	0.50
1:A:74:THR:HG21	3:A:334:HOH:O	2.12	0.50
1:A:87:LYS:CE	3:A:243:HOH:O	2.38	0.49
1:A:198:THR:CG2	3:A:399:HOH:O	2.59	0.49
2:D:304:ASP:OD1	2:D:304:ASP:N	2.46	0.49
1:C:205:HIS:HD2	1:C:208:SER:OG	1.96	0.49
1:A:27:TYR:CE1	1:A:98:ARG:HD2	2.49	0.48
2:B:288:MET:CE	2:B:296:HIS:HB2	2.30	0.48
1:C:219:ARG:CB	3:D:692:HOH:O	2.61	0.48
2:B:304:ASP:N	2:B:304:ASP:OD1	2.46	0.47
1:C:87:LYS:HA	1:C:87:LYS:HD3	1.71	0.47
2:D:292:LYS:O	2:D:310:SER:OG	2.27	0.47
1:C:192:SER:O	1:C:194:TRP:N	2.46	0.47
2:D:323:GLN:NE2	3:D:527:HOH:O	2.47	0.47
1:A:121:LYS:HB2	1:A:121:LYS:HE3	1.70	0.47
2:D:381:LEU:HD11	2:D:433:TRP:CE3	2.49	0.47
1:C:140:SER:CB	3:C:262:HOH:O	2.62	0.47
3:A:270:HOH:O	1:C:17:THR:HG21	2.13	0.46
2:B:390:PRO:O	2:B:445:HIS:HE1	1.99	0.46
1:A:214:LYS:HE3	3:B:653:HOH:O	2.13	0.46
1:A:191:SER:HA	1:A:192:SER:HA	1.63	0.46
2:B:432:GLN:O	2:B:436:HIS:HD2	1.99	0.46
2:D:419:LYS:HB2	3:D:537:HOH:O	2.14	0.46
2:B:339:LYS:HB2	2:B:339:LYS:NZ	2.31	0.46
2:B:430:SER:O	2:B:434:ARG:HG3	2.15	0.46
2:B:288:MET:HB3	2:B:298:THR:HG22	1.97	0.46
2:B:398:LYS:HB2	2:B:440:THR:HB	1.97	0.46
1:C:41:PRO:HG3	3:C:407:HOH:O	2.14	0.46
2:D:289:GLU:OE1	3:D:656:HOH:O	2.21	0.45
3:C:292:HOH:O	2:D:427:HIS:HE1	1.99	0.45
1:A:85:ASN:ND2	3:A:363:HOH:O	2.47	0.45
1:C:210:THR:HG22	3:C:355:HOH:O	2.17	0.44
2:D:432:GLN:O	2:D:436:HIS:HD2	2.00	0.44
2:D:373:GLU:CG	2:D:378:LYS:HB2	2.42	0.44
2:B:241:GLN:CD	2:B:348:GLY:H	2.26	0.44
1:A:104:LEU:HG	3:A:386:HOH:O	2.17	0.43
1:A:131:ALA:HB2	1:A:216:ILE:CG2	2.48	0.43
2:B:270:THR:HB	2:B:292:LYS:HD3	2.00	0.43
1:C:190:PRO:HA	1:C:191:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:THR:HG22	3:C:385:HOH:O	2.18	0.43
2:B:369:PRO:CG	2:B:379:ALA:HB1	2.49	0.43
2:D:288:MET:HE3	2:D:290:LEU:HB2	2.00	0.43
1:A:205:HIS:CD2	1:A:208:SER:OG	2.67	0.43
1:A:102:ASN:O	1:A:102:ASN:ND2	2.52	0.42
1:C:192:SER:HB2	3:C:346:HOH:O	2.19	0.42
1:A:148:VAL:HG11	1:A:156:VAL:HG11	2.01	0.42
1:A:27:TYR:CZ	1:A:98:ARG:HD2	2.55	0.41
2:B:288:MET:CE	2:B:296:HIS:HB3	2.50	0.41
2:D:290:LEU:HD23	2:D:315:ARG:HB3	2.02	0.41
1:C:6:GLN:NE2	1:C:112:GLY:H	2.19	0.41
2:D:365:THR:HG23	3:D:476:HOH:O	2.21	0.41
2:D:364:LEU:HD21	2:D:443:VAL:HG21	2.02	0.41
1:C:140:SER:C	1:C:191:SER:HG	2.26	0.40
2:D:305:ARG:HG3	2:D:320:SER:O	2.21	0.40
1:C:104:LEU:HD23	1:C:107:ALA:HB2	2.02	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)
3:B:577:HOH:O	3:C:437:HOH:O[2_756]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	214/220 (97%)	209 (98%)	4 (2%)	1 (0%)	24	16
1	C	214/220 (97%)	208 (97%)	4 (2%)	2 (1%)	14	6
2	B	200/218 (92%)	190 (95%)	9 (4%)	1 (0%)	24	16
2	D	199/218 (91%)	195 (98%)	3 (2%)	1 (0%)	24	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	827/876 (94%)	802 (97%)	20 (2%)	5 (1%)	21	13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	ARG
2	D	389	SER
2	B	339	LYS
1	C	191	SER
1	C	192	SER

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	185/186 (100%)	178 (96%)	7 (4%)	29	21
1	C	184/186 (99%)	175 (95%)	9 (5%)	22	14
2	B	179/191 (94%)	173 (97%)	6 (3%)	32	25
2	D	178/191 (93%)	168 (94%)	10 (6%)	19	11
All	All	726/754 (96%)	694 (96%)	32 (4%)	25	17

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	121	LYS
1	A	141	MET
1	A	177	GLN
1	A	191	SER
1	A	196	SER
1	A	197	GLN
2	B	281	LEU
2	B	304	ASP
2	B	339	LYS

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Mol	Chain	Res	Type
2	B	363	THR
2	B	391	SER
2	B	394	THR
1	C	2	ILE
1	C	98	ARG
1	C	102	ASN
1	C	104	LEU
1	C	121	LYS
1	C	141	MET
1	C	156	VAL
1	C	196	SER
1	C	197	GLN
2	D	257	SER
2	D	285	LYS
2	D	304	ASP
2	D	345	VAL
2	D	365	THR
2	D	381	LEU
2	D	389	SER
2	D	402	THR
2	D	419	LYS
2	D	451	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	6	GLN
1	A	102	ASN
1	A	139	ASN
1	A	170	HIS
1	A	202	ASN
1	A	205	HIS
2	B	241	GLN
2	B	321	ASN
2	B	357	GLN
2	B	436	HIS
2	B	445	HIS
1	C	6	GLN
1	C	177	GLN
1	C	197	GLN
1	C	202	ASN

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Mol	Chain	Res	Type
1	C	205	HIS
2	D	265	ASN
2	D	323	GLN
2	D	357	GLN
2	D	377	ASN
2	D	400	ASN
2	D	427	HIS
2	D	436	HIS
2	D	442	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	218/220 (99%)	-1.32	0 100 100	4, 13, 30, 38	0
1	C	218/220 (99%)	-1.31	0 100 100	5, 14, 30, 38	0
2	B	204/218 (93%)	-1.32	0 100 100	5, 14, 29, 36	0
2	D	203/218 (93%)	-1.30	0 100 100	4, 14, 28, 35	1 (0%)
All	All	843/876 (96%)	-1.31	0 100 100	4, 14, 30, 38	1 (0%)

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.