



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:37 PM UTC

PDB ID : 4TXS / pdb_00004txs
Title : An Ligand-observed Mass Spectrometry-based Approach Integrated into the
Fragment Based Lead Discovery Pipeline
Authors : Shui, W.; Yang, C.; Lin, J.; Chen, X.; Qin, S.; Chen, S.
Deposited on : 2014-07-07
Resolution : 2.78 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

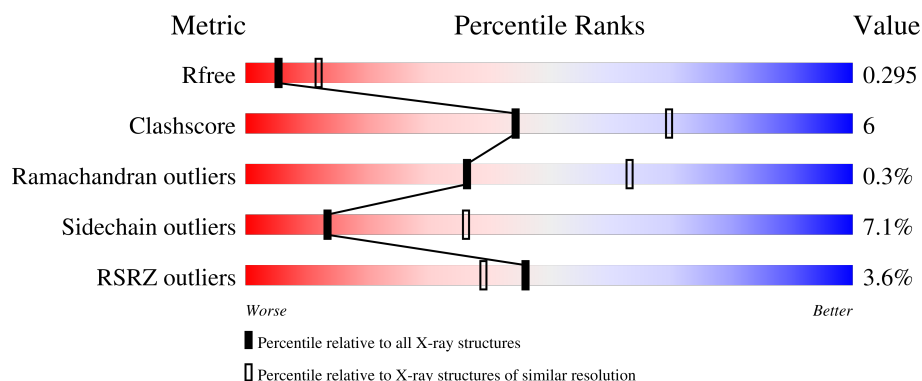
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	566	3% 79% 16% • •
1	B	566	4% 79% 15% • •
1	C	566	4% 75% 17% • •
1	D	566	3% 81% 12% • •

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	3AQ	D	601	-	-	X	-

2 Entry composition [i](#)

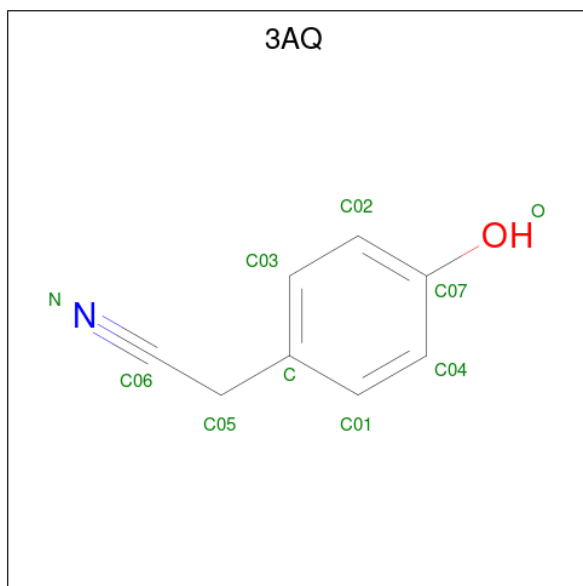
There are 2 unique types of molecules in this entry. The entry contains 16928 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	0	0
			4222	2664	744	783	31			
1	B	544	Total	C	N	O	S	0	0	0
			4222	2664	744	783	31			
1	C	544	Total	C	N	O	S	0	0	0
			4222	2664	744	783	31			
1	D	544	Total	C	N	O	S	0	0	0
			4222	2664	744	783	31			

- Molecule 2 is (4-hydroxyphenyl)acetonitrile (CCD ID: 3AQ) (formula: C₈H₇NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	8	1	1		
2	B	1	Total	C	N	O	0	0
			10	8	1	1		

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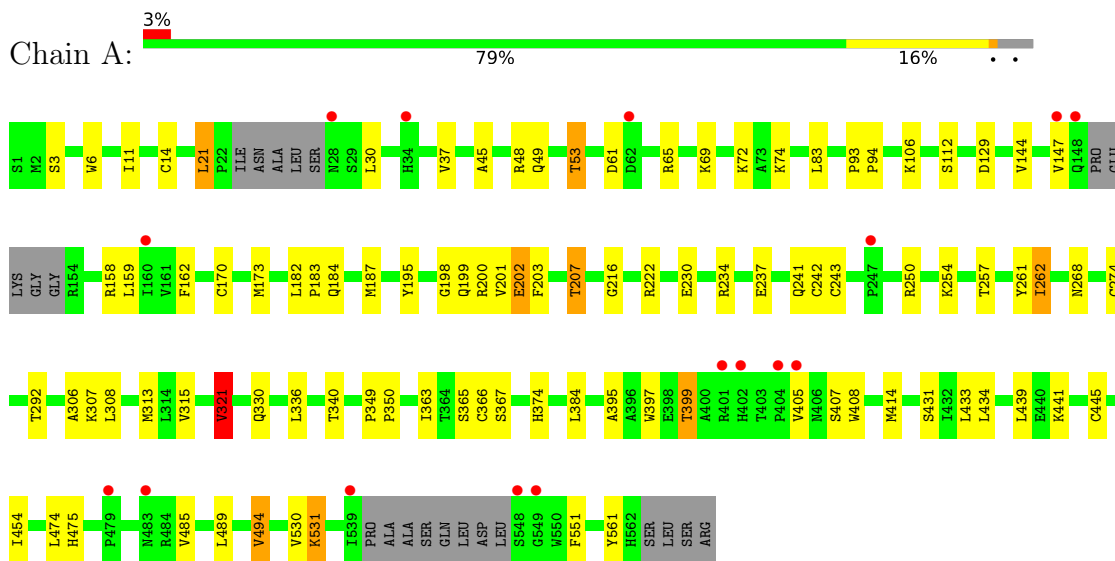
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			10	8	1	1		
2	D	1	Total	C	N	O	0	0
			10	8	1	1		

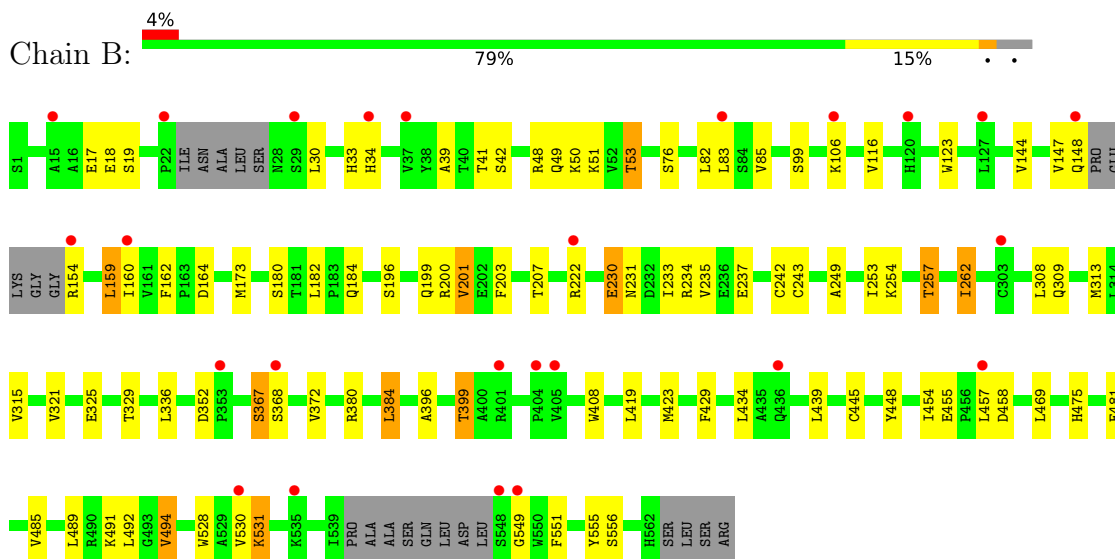
3 Residue-property plots [i](#)

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: Polypeptide

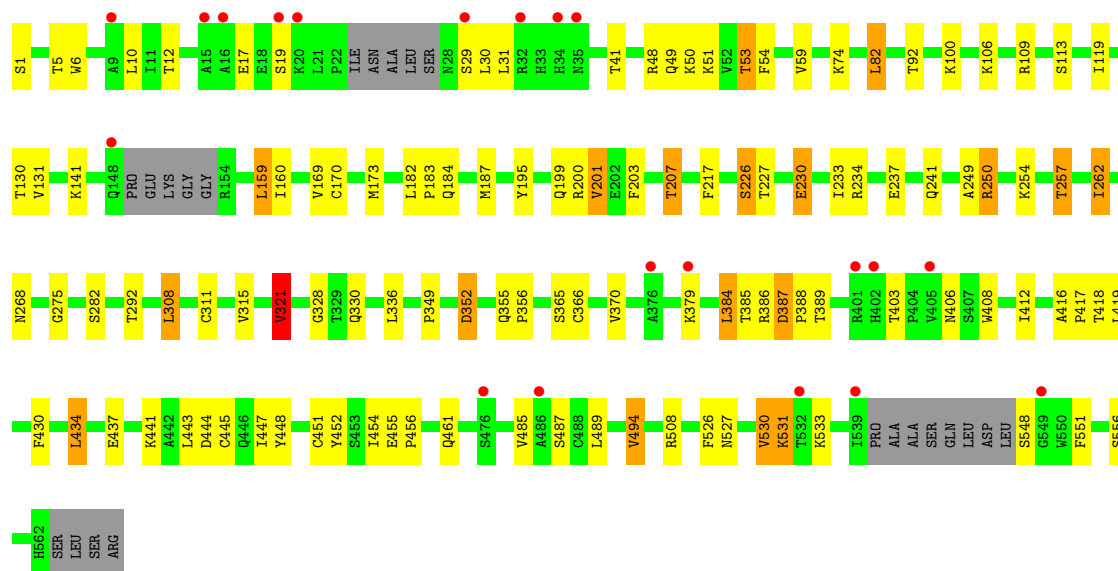


- Molecule 1: Polypeptide



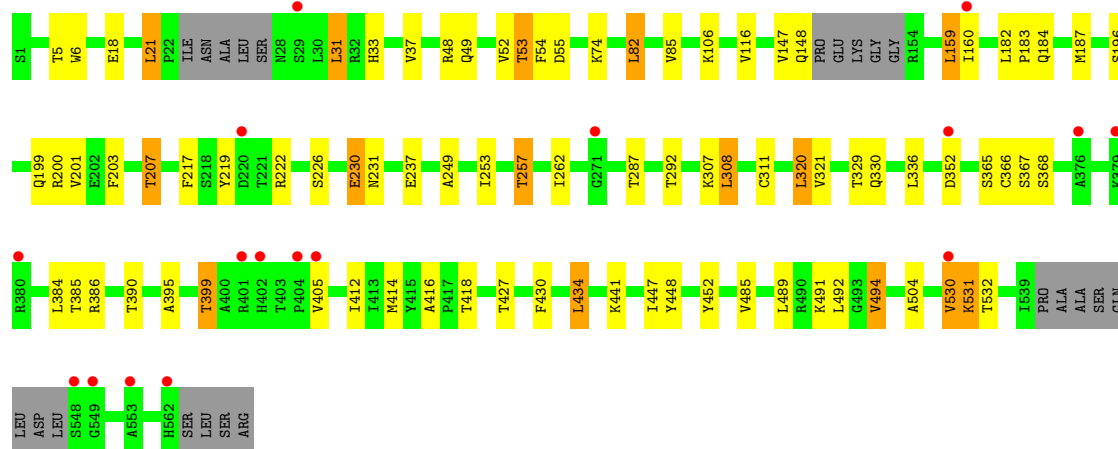
- Molecule 1: Polypeptide

Chain C: 



• Molecule 1: Polyprotein

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.18Å 102.08Å 251.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.69 – 2.78 45.69 – 2.78	Depositor EDS
% Data completeness (in resolution range)	95.2 (45.69-2.78) 95.2 (45.69-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.59 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0049, REFMAC 5.8.0049	Depositor
R, R_{free}	0.220 , 0.294 0.224 , 0.295	Depositor DCC
R_{free} test set	3228 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 15.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.079 for k,h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16928	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3AQ

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	0.79	1/4313 (0.0%)	1.00	5/5852 (0.1%)
1	B	0.77	0/4313	1.00	8/5852 (0.1%)
1	C	0.81	0/4313	1.05	8/5852 (0.1%)
1	D	0.80	0/4313	1.01	5/5852 (0.1%)
All	All	0.79	1/17252 (0.0%)	1.02	26/23408 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	PRO	CA-C	5.07	1.54	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	131	VAL	N-CA-C	7.67	117.68	111.62
1	D	352	ASP	CA-C-N	-6.81	114.76	119.66
1	D	352	ASP	C-N-CA	-6.81	114.76	119.66
1	C	328	GLY	N-CA-C	-6.78	105.51	111.95
1	C	321	VAL	CB-CA-C	-6.40	100.44	110.69
1	C	387	ASP	N-CA-C	-6.08	101.92	109.64
1	D	390	THR	CA-C-N	-5.96	112.43	119.05
1	D	390	THR	C-N-CA	-5.96	112.43	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	THR	N-CA-C	5.82	117.63	111.28
1	B	475	HIS	CA-C-N	-5.72	115.31	123.20
1	B	475	HIS	C-N-CA	-5.72	115.31	123.20
1	A	349	PRO	CA-C-N	5.71	125.61	119.85
1	A	349	PRO	C-N-CA	5.71	125.61	119.85
1	B	201	VAL	CB-CA-C	-5.63	104.53	112.14
1	A	321	VAL	CB-CA-C	-5.63	101.83	110.50
1	C	352	ASP	CA-C-N	-5.55	114.66	120.38
1	C	352	ASP	C-N-CA	-5.55	114.66	120.38
1	B	230	GLU	N-CA-C	-5.53	105.33	111.36
1	D	287	THR	N-CA-C	5.47	116.92	111.07
1	B	162	PHE	N-CA-C	5.32	114.97	108.11
1	C	530	VAL	N-CA-C	5.31	115.53	110.53
1	A	162	PHE	N-CA-C	5.30	114.95	108.11
1	B	352	ASP	CA-C-N	-5.18	115.05	120.38
1	B	352	ASP	C-N-CA	-5.18	115.05	120.38
1	A	475	HIS	N-CA-C	5.14	121.76	110.80
1	C	201	VAL	CB-CA-C	-5.07	105.23	112.22

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	548	SER	Peptide

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	4222	0	4212	48	0
1	B	4222	0	4212	40	0
1	C	4222	0	4212	61	0
1	D	4222	0	4212	54	0
2	A	10	0	7	1	0
2	B	10	0	7	0	0
2	C	10	0	6	1	0
2	D	10	0	7	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16928	0	16875	203	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 6.

All (203) 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:49:GLN:O	1:C:53:THR:HG22	1.58	1.03
1:D:49:GLN:O	1:D:53:THR:HG23	1.64	0.96
1:B:49:GLN:O	1:B:53:THR:HG22	1.66	0.93
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.54	0.89
1:D:203:PHE:O	1:D:207:THR:HG23	1.71	0.89
1:B:203:PHE:O	1:B:207:THR:HG23	1.72	0.89
1:B:49:GLN:O	1:B:53:THR:CG2	2.21	0.88
1:B:253:ILE:O	1:B:257:THR:HG23	1.75	0.86
1:A:340:THR:HG23	1:A:350:PRO:HG3	1.62	0.82
1:C:49:GLN:O	1:C:53:THR:CG2	2.30	0.79
1:D:6:TRP:HE1	1:D:53:THR:HG21	1.46	0.79
1:A:49:GLN:O	1:A:53:THR:CG2	2.31	0.78
1:C:203:PHE:O	1:C:207:THR:HG23	1.82	0.78
1:A:395:ALA:O	1:A:399:THR:HG22	1.82	0.77
1:D:489:LEU:HA	1:D:494:VAL:HG13	1.68	0.75
1:D:253:ILE:O	1:D:257:THR:HG23	1.88	0.74
1:D:49:GLN:O	1:D:53:THR:CG2	2.36	0.74
1:C:201:VAL:HG22	1:C:384:LEU:HD13	1.70	0.73
1:B:196:SER:H	1:B:199:GLN:HE21	1.35	0.73
1:C:1:SER:OG	1:C:230:GLU:OE1	2.08	0.70
1:A:48:ARG:HG2	1:A:159:LEU:HD13	1.73	0.69
1:C:82:LEU:HD13	1:C:249:ALA:HB2	1.74	0.69
1:C:48:ARG:HG2	1:C:159:LEU:HD13	1.76	0.68
1:D:321:VAL:CG2	1:D:365:SER:HB3	2.26	0.66
1:A:6:TRP:HE1	1:A:53:THR:HG21	1.63	0.63
1:A:257:THR:HG22	1:A:261:TYR:HD2	1.62	0.63
1:A:414:MET:HE3	2:A:601:3AQ:N	2.13	0.63
1:D:21:LEU:CD2	1:D:37:VAL:HB	2.29	0.63
1:A:203:PHE:O	1:A:207:THR:HG23	1.99	0.63
1:D:48:ARG:HG2	1:D:159:LEU:HD13	1.82	0.62
1:C:268:ASN:OD1	1:C:268:ASN:C	2.43	0.61
1:B:180:SER:OG	1:B:555:TYR:OH	2.17	0.61
1:C:448:TYR:CE2	1:C:551:PHE:HD1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:CYS:SG	1:A:454:ILE:HD12	2.41	0.60
1:D:530:VAL:O	1:D:531:LYS:HB3	2.00	0.60
1:D:321:VAL:HG21	1:D:365:SER:HB3	1.82	0.60
1:C:385:THR:OG1	1:C:386:ARG:N	2.35	0.59
1:C:160:ILE:HD12	1:C:282:SER:OG	2.02	0.59
1:D:187:MET:HE1	1:D:292:THR:HG22	1.84	0.59
1:D:237:GLU:HG3	1:D:257:THR:HG21	1.84	0.59
1:A:485:VAL:O	1:A:489:LEU:HG	2.03	0.59
1:D:321:VAL:CG2	1:D:365:SER:CB	2.81	0.59
1:A:49:GLN:O	1:A:53:THR:HG22	2.01	0.58
1:D:414:MET:HE3	2:D:601:3AQ:H5	1.85	0.58
1:A:49:GLN:O	1:A:53:THR:HG23	2.03	0.57
1:D:82:LEU:HD13	1:D:249:ALA:HB2	1.86	0.57
1:B:396:ALA:O	1:B:399:THR:HG22	2.04	0.57
1:C:187:MET:HE1	1:C:292:THR:HG22	1.86	0.57
1:C:170:CYS:HA	1:C:173:MET:HE3	1.87	0.56
1:A:198:GLY:O	1:A:202:GLU:HB2	2.05	0.56
1:C:447:ILE:HB	1:C:452:TYR:CE2	2.41	0.56
1:A:48:ARG:CG	1:A:159:LEU:HD13	2.36	0.56
1:D:33:HIS:HD2	1:D:491:LYS:O	1.88	0.56
1:D:321:VAL:HG21	1:D:365:SER:CB	2.34	0.56
1:C:430:PHE:O	1:C:434:LEU:HB2	2.05	0.55
1:C:31:LEU:HD12	1:C:31:LEU:O	2.06	0.55
1:D:414:MET:CE	2:D:601:3AQ:C05	2.84	0.55
1:B:455:GLU:HB2	1:B:458:ASP:OD2	2.06	0.55
1:B:123:TRP:CE3	1:B:173:MET:HE3	2.41	0.55
1:C:241:GLN:OE1	1:C:250:ARG:HG2	2.06	0.55
1:C:485:VAL:O	1:C:489:LEU:HG	2.07	0.55
1:B:445:CYS:SG	1:B:454:ILE:HD12	2.46	0.55
1:A:489:LEU:HA	1:A:494:VAL:HG13	1.89	0.55
1:D:201:VAL:HG22	1:D:384:LEU:HD13	1.88	0.55
1:C:530:VAL:O	1:C:531:LYS:CB	2.54	0.54
1:D:485:VAL:O	1:D:489:LEU:HG	2.07	0.54
1:B:196:SER:H	1:B:199:GLN:NE2	2.05	0.54
1:B:237:GLU:CG	1:B:257:THR:HG21	2.38	0.54
1:A:11:ILE:HD12	1:A:45:ALA:HB1	1.90	0.53
1:A:21:LEU:CD2	1:A:37:VAL:HB	2.37	0.53
1:A:72:LYS:HG2	1:A:242:CYS:SG	2.48	0.53
1:A:292:THR:HG23	1:A:315:VAL:HG12	1.89	0.53
1:A:195:TYR:HA	1:A:199:GLN:HE21	1.74	0.53
1:C:237:GLU:HG3	1:C:257:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:VAL:HG22	1:C:365:SER:CB	2.38	0.53
1:C:527:ASN:ND2	1:C:533:LYS:HB3	2.24	0.53
1:D:196:SER:H	1:D:199:GLN:HE21	1.56	0.53
1:D:414:MET:CE	2:D:601:3AQ:H6	2.39	0.53
1:B:182:LEU:HD13	1:B:243:CYS:SG	2.49	0.52
1:D:147:VAL:HG12	1:D:148:GLN:HG2	1.91	0.52
1:B:196:SER:OG	1:B:199:GLN:HG3	2.09	0.52
1:C:308:LEU:HB3	1:C:311:CYS:SG	2.50	0.52
1:A:201:VAL:HG22	1:A:384:LEU:HD13	1.91	0.51
1:A:3:SER:OG	1:A:53:THR:HA	2.11	0.51
1:B:231:ASN:O	1:B:235:VAL:HG23	2.11	0.51
1:A:374:HIS:O	1:A:474:LEU:HA	2.10	0.51
1:C:92:THR:O	1:C:109:ARG:NH1	2.41	0.51
1:D:395:ALA:O	1:D:399:THR:HG22	2.11	0.51
1:D:187:MET:HE1	1:D:292:THR:CG2	2.41	0.51
1:B:99:SER:HA	1:B:164:ASP:OD1	2.10	0.51
1:B:33:HIS:HD2	1:B:491:LYS:O	1.94	0.50
1:D:237:GLU:CG	1:D:257:THR:HG21	2.41	0.50
1:D:217:PHE:CD1	1:D:336:LEU:HD21	2.46	0.50
1:D:447:ILE:HB	1:D:452:TYR:CE2	2.47	0.50
1:D:530:VAL:O	1:D:531:LYS:CB	2.60	0.50
1:D:412:ILE:O	1:D:416:ALA:N	2.45	0.50
1:D:414:MET:CE	2:D:601:3AQ:H5	2.42	0.49
1:A:321:VAL:HG22	1:A:365:SER:HB2	1.95	0.49
1:B:48:ARG:HG2	1:B:159:LEU:HD13	1.93	0.49
1:C:419:LEU:HD23	1:C:485:VAL:HG21	1.94	0.49
1:B:372:VAL:HG13	1:B:372:VAL:O	2.13	0.49
1:B:201:VAL:HG22	1:B:384:LEU:HD13	1.94	0.48
1:C:445:CYS:SG	1:C:454:ILE:HD12	2.53	0.48
1:D:200:ARG:HD3	1:D:384:LEU:HD21	1.96	0.48
1:B:309:GLN:HB2	1:B:325:GLU:HB2	1.96	0.48
1:D:237:GLU:HG3	1:D:257:THR:CG2	2.43	0.48
1:D:489:LEU:HA	1:D:494:VAL:CG1	2.40	0.48
1:B:30:LEU:O	1:B:494:VAL:HB	2.14	0.47
1:B:485:VAL:O	1:B:489:LEU:HG	2.14	0.47
1:A:182:LEU:HD13	1:A:243:CYS:SG	2.54	0.47
1:C:489:LEU:HD22	1:C:494:VAL:HG21	1.96	0.47
1:C:489:LEU:HD22	1:C:494:VAL:CG2	2.45	0.47
1:B:237:GLU:HG3	1:B:257:THR:HG21	1.95	0.47
1:C:6:TRP:HE1	1:C:53:THR:HG21	1.80	0.47
1:C:527:ASN:HD21	1:C:533:LYS:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:489:LEU:CA	1:D:494:VAL:HG13	2.41	0.47
1:C:366:CYS:HB3	2:C:601:3AQ:C01	2.45	0.47
1:B:234:ARG:HG2	1:B:262:ILE:HD11	1.97	0.47
1:B:17:GLU:HB3	1:B:41:THR:HG22	1.97	0.46
1:A:306:ALA:O	1:A:307:LYS:C	2.57	0.46
1:C:530:VAL:O	1:C:531:LYS:HB3	2.14	0.46
1:A:414:MET:HE1	1:A:551:PHE:HE1	1.80	0.46
1:C:187:MET:SD	1:C:292:THR:HG22	2.56	0.46
1:C:455:GLU:O	1:C:456:PRO:C	2.58	0.45
1:D:52:VAL:HB	1:D:226:SER:OG	2.17	0.45
1:B:85:VAL:HG11	1:B:116:VAL:HG13	1.98	0.45
1:B:39:ALA:HB2	1:B:144:VAL:HG22	1.98	0.45
1:C:195:TYR:HA	1:C:199:GLN:HE21	1.82	0.45
1:D:427:THR:HG23	1:D:504:ALA:HA	1.99	0.45
1:B:439:LEU:HB3	1:B:457:LEU:HD21	1.98	0.45
1:C:10:LEU:O	1:C:12:THR:HG23	2.16	0.45
1:A:30:LEU:O	1:A:494:VAL:HB	2.16	0.45
1:B:233:ILE:HG22	1:B:262:ILE:HD12	1.98	0.45
1:D:321:VAL:HG23	1:D:365:SER:CB	2.47	0.45
1:C:217:PHE:CD1	1:C:336:LEU:HD21	2.52	0.45
1:A:237:GLU:HG3	1:A:257:THR:HG21	2.00	0.44
1:B:423:MET:HA	1:B:528:TRP:CZ2	2.52	0.44
1:C:385:THR:HB	1:C:418:THR:HG22	1.98	0.44
1:D:230:GLU:O	1:D:231:ASN:C	2.60	0.44
1:D:447:ILE:O	1:D:448:TYR:C	2.60	0.44
1:B:530:VAL:O	1:B:531:LYS:CB	2.65	0.44
1:D:219:TYR:HB3	1:D:320:LEU:HD23	1.99	0.44
1:A:187:MET:HE1	1:A:292:THR:CG2	2.47	0.44
1:A:433:LEU:HB3	1:A:439:LEU:HD23	2.00	0.44
1:C:201:VAL:HG13	1:C:370:VAL:HG22	2.00	0.44
1:D:21:LEU:HD23	1:D:37:VAL:HB	1.99	0.44
1:B:448:TYR:CE2	1:B:551:PHE:HD1	2.36	0.43
1:A:170:CYS:HA	1:A:173:MET:HE3	1.99	0.43
1:C:387:ASP:HA	1:C:388:PRO:HD3	1.84	0.43
1:D:385:THR:HB	1:D:418:THR:HG22	1.99	0.43
1:B:408:TRP:CD1	1:B:429:PHE:CE1	3.07	0.43
1:A:94:PRO:HD3	1:A:561:TYR:CD1	2.53	0.43
1:A:530:VAL:O	1:A:531:LYS:HB2	2.19	0.43
1:C:119:ILE:HD13	1:C:169:VAL:HG11	2.00	0.43
1:D:385:THR:OG1	1:D:386:ARG:N	2.51	0.43
1:A:203:PHE:O	1:A:207:THR:CG2	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:VAL:HG22	1:A:365:SER:CB	2.49	0.43
1:C:30:LEU:O	1:C:494:VAL:HB	2.19	0.43
1:C:355:GLN:HA	1:C:356:PRO:HD3	1.91	0.43
1:D:54:PHE:HD1	1:D:55:ASP:O	2.02	0.43
1:A:187:MET:HE1	1:A:292:THR:HG22	2.00	0.43
1:B:76:SER:HA	1:B:242:CYS:O	2.18	0.43
1:D:321:VAL:HG23	1:D:365:SER:HB2	2.01	0.43
1:B:419:LEU:HD23	1:B:485:VAL:HG21	2.01	0.42
1:A:216:GLY:HA3	1:A:363:ILE:HD11	2.01	0.42
1:C:17:GLU:OE1	1:C:41:THR:HB	2.19	0.42
1:D:196:SER:H	1:D:199:GLN:NE2	2.16	0.42
1:B:48:ARG:O	1:B:49:GLN:C	2.62	0.42
1:C:48:ARG:CG	1:C:159:LEU:HD13	2.48	0.42
1:C:201:VAL:CG2	1:C:384:LEU:HD22	2.50	0.42
1:C:54:PHE:CZ	1:C:226:SER:HB3	2.55	0.42
1:B:481:GLU:O	1:B:485:VAL:HG23	2.20	0.42
1:A:340:THR:CG2	1:A:350:PRO:HG3	2.42	0.42
1:C:387:ASP:OD2	1:C:389:THR:OG1	2.16	0.42
1:C:444:ASP:HB3	1:C:451:CYS:SG	2.60	0.42
1:A:61:ASP:O	1:A:65:ARG:HG3	2.19	0.41
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.60	0.41
1:C:200:ARG:HD3	1:C:384:LEU:HD21	2.02	0.41
1:C:234:ARG:HG3	1:C:262:ILE:HD11	2.03	0.41
1:D:85:VAL:HG11	1:D:116:VAL:HG22	2.01	0.41
1:D:308:LEU:HB3	1:D:311:CYS:SG	2.61	0.41
1:C:227:THR:HG21	1:C:349:PRO:HD2	2.02	0.41
1:C:444:ASP:HA	1:C:452:TYR:O	2.20	0.41
1:C:233:ILE:HB	1:C:262:ILE:HD12	2.02	0.41
1:C:321:VAL:HG22	1:C:365:SER:HB3	2.01	0.41
1:C:416:ALA:N	1:C:417:PRO:CD	2.84	0.41
1:D:182:LEU:HB3	1:D:183:PRO:HD3	2.02	0.41
1:D:366:CYS:O	1:D:368:SER:N	2.53	0.41
1:C:408:TRP:HE3	1:C:412:ILE:HD12	1.86	0.41
1:A:200:ARG:HD3	1:A:384:LEU:HD21	2.02	0.41
1:A:234:ARG:HG3	1:A:262:ILE:HD11	2.03	0.41
1:A:182:LEU:HB3	1:A:183:PRO:HD3	2.03	0.41
1:A:129:ASP:OD1	1:A:129:ASP:C	2.64	0.41
1:A:407:SER:O	1:A:408:TRP:C	2.62	0.41
1:C:182:LEU:N	1:C:183:PRO:CD	2.84	0.40
1:D:430:PHE:O	1:D:434:LEU:HB2	2.20	0.40
1:B:200:ARG:HD3	1:B:384:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:ARG:HG3	1:C:526:PHE:HB2	2.03	0.40
1:A:144:VAL:HG21	1:A:397:TRP:CG	2.57	0.40
1:C:5:THR:O	1:C:275:GLY:HA3	2.21	0.40
1:C:406:ASN:ND2	1:C:443:LEU:HB3	2.37	0.40
1:A:241:GLN:OE1	1:A:250:ARG:HG2	2.22	0.40
1:D:31:LEU:C	1:D:31:LEU:HD12	2.46	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	536/566 (95%)	509 (95%)	26 (5%)	1 (0%)	43	70
1	B	536/566 (95%)	506 (94%)	27 (5%)	3 (1%)	21	47
1	C	536/566 (95%)	508 (95%)	27 (5%)	1 (0%)	43	70
1	D	536/566 (95%)	509 (95%)	25 (5%)	2 (0%)	30	57
All	All	2144/2264 (95%)	2032 (95%)	105 (5%)	7 (0%)	36	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	531	LYS
1	C	531	LYS
1	D	531	LYS
1	B	531	LYS
1	B	367	SER
1	D	367	SER
1	B	549	GLY

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	460/482 (95%)	430 (94%)	30 (6%)	15	40
1	B	460/482 (95%)	425 (92%)	35 (8%)	12	33
1	C	460/482 (95%)	423 (92%)	37 (8%)	11	31
1	D	460/482 (95%)	431 (94%)	29 (6%)	16	41
All	All	1840/1928 (95%)	1709 (93%)	131 (7%)	13	36

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	CYS
1	A	21	LEU
1	A	53	THR
1	A	69	LYS
1	A	74	LYS
1	A	83	LEU
1	A	106	LYS
1	A	112	SER
1	A	147	VAL
1	A	158	ARG
1	A	184	GLN
1	A	202	GLU
1	A	207	THR
1	A	222	ARG
1	A	230	GLU
1	A	254	LYS
1	A	262	ILE
1	A	308	LEU
1	A	313	MET
1	A	321	VAL
1	A	330	GLN
1	A	336	LEU
1	A	366	CYS
1	A	367	SER

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Mol	Chain	Res	Type
1	A	399	THR
1	A	405	VAL
1	A	431	SER
1	A	434	LEU
1	A	441	LYS
1	A	494	VAL
1	B	18	GLU
1	B	19	SER
1	B	34	HIS
1	B	42	SER
1	B	50	LYS
1	B	51	LYS
1	B	53	THR
1	B	83	LEU
1	B	106	LYS
1	B	147	VAL
1	B	148	GLN
1	B	154	ARG
1	B	159	LEU
1	B	160	ILE
1	B	184	GLN
1	B	222	ARG
1	B	230	GLU
1	B	254	LYS
1	B	257	THR
1	B	262	ILE
1	B	308	LEU
1	B	313	MET
1	B	315	VAL
1	B	321	VAL
1	B	336	LEU
1	B	367	SER
1	B	368	SER
1	B	380	ARG
1	B	384	LEU
1	B	399	THR
1	B	434	LEU
1	B	469	LEU
1	B	492	LEU
1	B	494	VAL
1	B	556	SER
1	C	19	SER

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Mol	Chain	Res	Type
1	C	29	SER
1	C	50	LYS
1	C	51	LYS
1	C	53	THR
1	C	59	VAL
1	C	74	LYS
1	C	82	LEU
1	C	100	LYS
1	C	106	LYS
1	C	113	SER
1	C	130	THR
1	C	141	LYS
1	C	159	LEU
1	C	184	GLN
1	C	207	THR
1	C	226	SER
1	C	230	GLU
1	C	250	ARG
1	C	254	LYS
1	C	257	THR
1	C	262	ILE
1	C	308	LEU
1	C	315	VAL
1	C	321	VAL
1	C	330	GLN
1	C	352	ASP
1	C	379	LYS
1	C	384	LEU
1	C	403	THR
1	C	434	LEU
1	C	437	GLU
1	C	441	LYS
1	C	461	GLN
1	C	487	SER
1	C	494	VAL
1	C	556	SER
1	D	5	THR
1	D	18	GLU
1	D	21	LEU
1	D	31	LEU
1	D	53	THR
1	D	74	LYS

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Mol	Chain	Res	Type
1	D	82	LEU
1	D	106	LYS
1	D	159	LEU
1	D	160	ILE
1	D	184	GLN
1	D	207	THR
1	D	222	ARG
1	D	230	GLU
1	D	257	THR
1	D	262	ILE
1	D	307	LYS
1	D	308	LEU
1	D	320	LEU
1	D	329	THR
1	D	330	GLN
1	D	399	THR
1	D	405	VAL
1	D	434	LEU
1	D	441	LYS
1	D	492	LEU
1	D	494	VAL
1	D	530	VAL
1	D	532	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	58	GLN
1	A	184	GLN
1	A	199	GLN
1	A	428	HIS
1	A	502	HIS
1	A	562	HIS
1	B	33	HIS
1	B	58	GLN
1	B	199	GLN
1	B	273	ASN
1	B	355	GLN
1	B	374	HIS
1	B	502	HIS
1	B	527	ASN

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Mol	Chain	Res	Type
1	C	120	HIS
1	C	184	GLN
1	C	199	GLN
1	C	309	GLN
1	C	402	HIS
1	C	406	ASN
1	C	428	HIS
1	C	502	HIS
1	C	527	ASN
1	D	28	ASN
1	D	33	HIS
1	D	58	GLN
1	D	120	HIS
1	D	199	GLN
1	D	273	ASN
1	D	402	HIS

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](#)

4 ligands are modelled in this entry.

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	3AQ	B	601	-	10,10,10	1.06	1 (10%)	12,12,12	1.37	1 (8%)
2	3AQ	A	601	-	10,10,10	0.81	0	12,12,12	1.22	2 (16%)
2	3AQ	C	601	-	10,10,10	0.85	1 (10%)	12,12,12	0.78	0
2	3AQ	D	601	-	10,10,10	0.62	0	12,12,12	1.27	2 (16%)

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	3AQ	B	601	-	-	0/2/3/3	0/1/1/1
2	3AQ	A	601	-	-	0/2/3/3	0/1/1/1
2	3AQ	C	601	-	-	0/2/3/3	0/1/1/1
2	3AQ	D	601	-	-	0/2/3/3	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	3AQ	C05-C06	2.44	1.50	1.46
2	C	601	3AQ	C05-C06	2.10	1.50	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	3AQ	C05-C06-N	-3.80	166.59	177.87
2	D	601	3AQ	C-C05-C06	3.06	119.42	113.33
2	D	601	3AQ	C05-C06-N	-2.68	169.94	177.87
2	A	601	3AQ	C05-C-C01	2.14	125.25	120.42
2	A	601	3AQ	C05-C-C03	-2.10	115.67	120.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	3AQ	1	0
2	C	601	3AQ	1	0
2	D	601	3AQ	4	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	544/566 (96%)	0.30	16 (2%) 53 46	19, 32, 51, 77	0
1	B	544/566 (96%)	0.31	25 (4%) 37 31	18, 31, 53, 84	0
1	C	544/566 (96%)	0.31	20 (3%) 45 38	18, 32, 54, 78	0
1	D	544/566 (96%)	0.27	17 (3%) 51 44	19, 31, 51, 87	0
All	All	2176/2264 (96%)	0.30	78 (3%) 46 39	18, 32, 53, 87	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	549	GLY	5.3
1	B	353	PRO	4.3
1	A	549	GLY	4.2
1	B	535	LYS	4.2
1	C	379	LYS	4.2
1	C	15	ALA	4.1
1	B	404	PRO	4.0
1	B	548	SER	3.9
1	A	548	SER	3.6
1	A	405	VAL	3.5
1	D	402	HIS	3.5
1	A	402	HIS	3.4
1	C	405	VAL	3.4
1	B	29	SER	3.4
1	D	271	GLY	3.4
1	B	530	VAL	3.3
1	D	160	ILE	3.3
1	D	404	PRO	3.2
1	C	34	HIS	3.2
1	A	404	PRO	3.1
1	C	16	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	28	ASN	3.0
1	D	549	GLY	3.0
1	B	303	CYS	3.0
1	B	148	GLN	2.9
1	C	20	LYS	2.9
1	C	549	GLY	2.8
1	C	29	SER	2.8
1	D	548	SER	2.7
1	D	405	VAL	2.7
1	A	539	ILE	2.7
1	D	352	ASP	2.7
1	B	160	ILE	2.7
1	A	401	ARG	2.7
1	D	220	ASP	2.7
1	C	402	HIS	2.6
1	B	106	LYS	2.6
1	A	247	PRO	2.6
1	C	35	ASN	2.6
1	A	62	ASP	2.6
1	A	148	GLN	2.5
1	D	376	ALA	2.5
1	C	476	SER	2.4
1	D	530	VAL	2.4
1	A	34	HIS	2.4
1	A	147	VAL	2.3
1	B	127	LEU	2.3
1	A	483	ASN	2.3
1	B	368	SER	2.3
1	D	29	SER	2.3
1	C	148	GLN	2.3
1	D	553	ALA	2.3
1	C	401	ARG	2.3
1	D	380	ARG	2.3
1	A	160	ILE	2.2
1	C	486	ALA	2.2
1	C	32	ARG	2.2
1	B	34	HIS	2.2
1	B	37	VAL	2.2
1	B	405	VAL	2.2
1	B	15	ALA	2.1
1	B	222	ARG	2.1
1	B	401	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	83	LEU	2.1
1	B	457	LEU	2.1
1	C	539	ILE	2.1
1	D	379	LYS	2.1
1	D	401	ARG	2.1
1	B	22	PRO	2.1
1	C	9	ALA	2.1
1	C	19	SER	2.1
1	C	376	ALA	2.1
1	C	532	THR	2.1
1	A	479	PRO	2.1
1	B	120	HIS	2.0
1	D	562	HIS	2.0
1	B	154	ARG	2.0
1	B	436	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	3AQ	B	601	10/10	0.68	0.27	63,66,71,75	0
2	3AQ	A	601	10/10	0.72	0.24	49,62,72,72	0
2	3AQ	C	601	10/10	0.76	0.27	58,62,67,68	0
2	3AQ	D	601	10/10	0.83	0.23	53,59,61,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.