



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:05 PM UTC

PDB ID : 4TY8 / pdb_00004ty8
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 : 2014-07-08
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

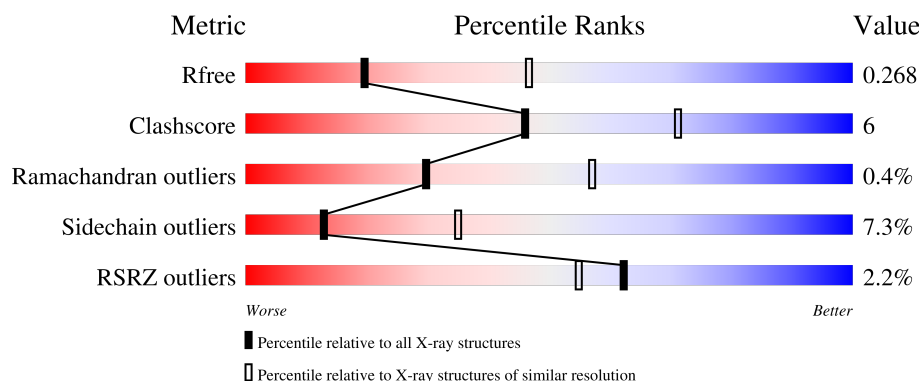
1 Overall quality at a glance

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	 2% 78% 15% . .
1	C	566	 % 81% 13% . .
1	D	566	 2% 78% 16% . .
2	B	566	 2% 81% 13% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16942 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	C	545	Total	C	N	O	S	0	0	0
			4229	2669	745	784	31			
1	D	546	Total	C	N	O	S	0	0	0
			4234	2672	746	785	31			

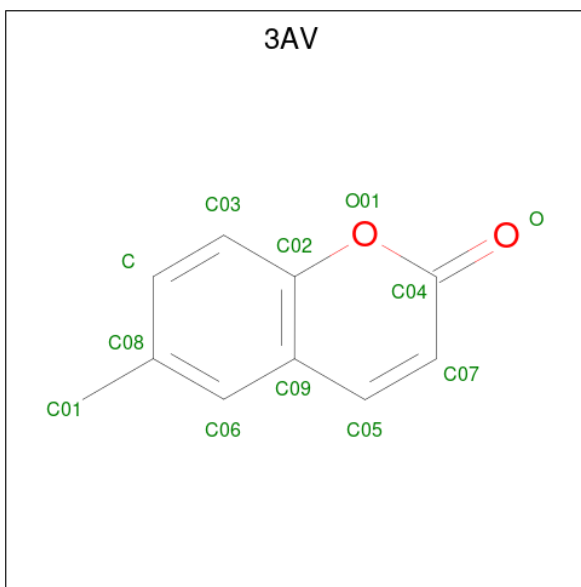
- Molecule 2 is a protein called Polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	547	Total	C	N	O	S	0	0	0
			4233	2669	746	786	32			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	550	MET	TRP	engineered mutation	UNP D0PY27

- Molecule 3 is 6-methyl-2H-chromen-2-one (CCD ID: 3AV) (formula: C₁₀H₈O₂).

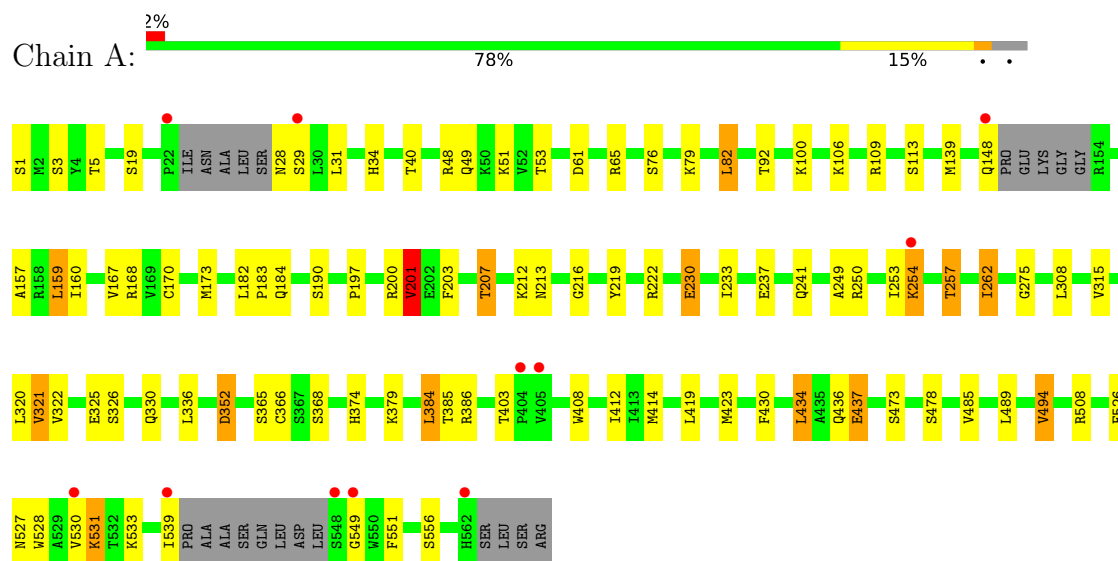


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	10	2		
3	B	1	Total	C	O	0	0
			12	10	2		

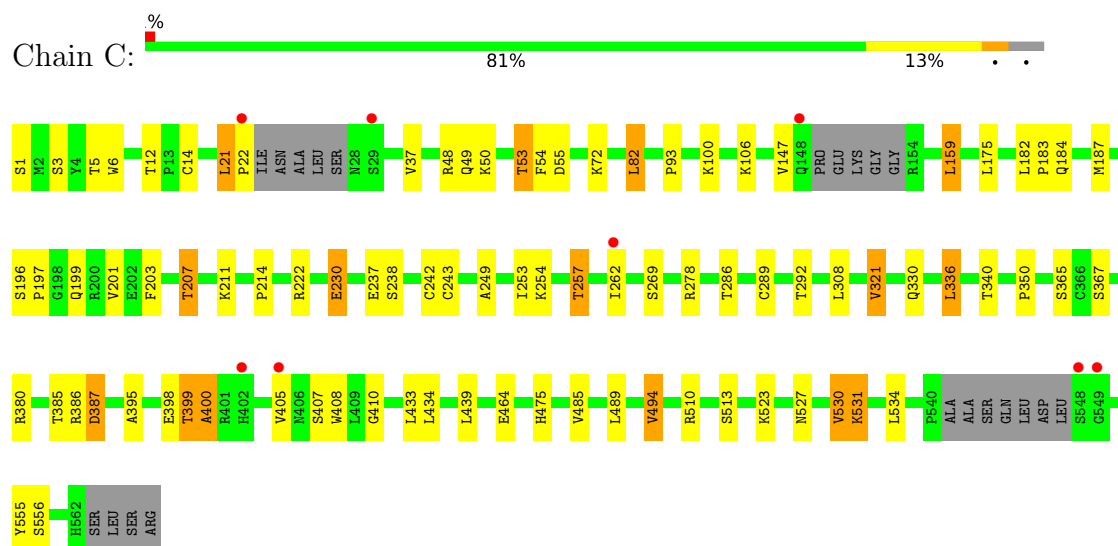
3 Residue-property plots

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.

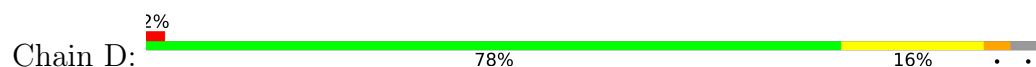
• Molecule 1: Polyprotein

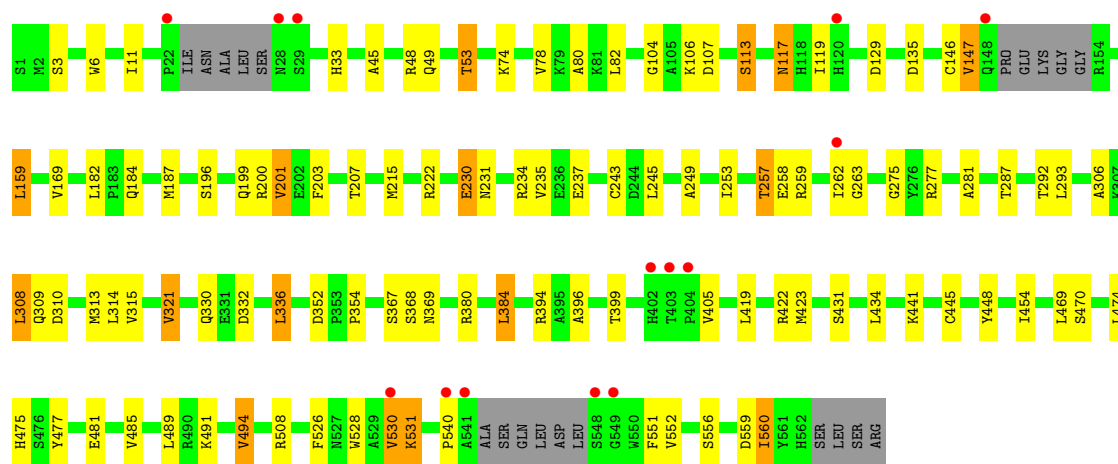


• Molecule 1: Polyprotein

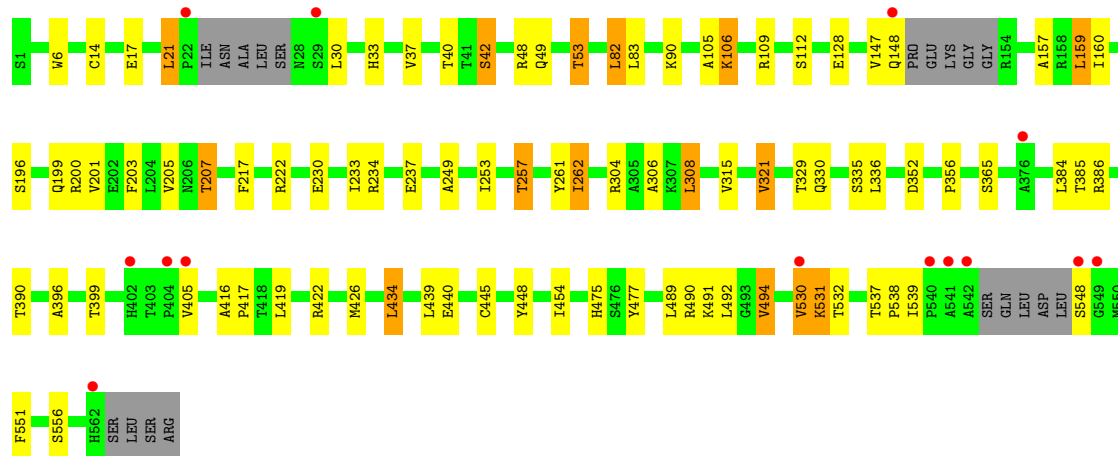
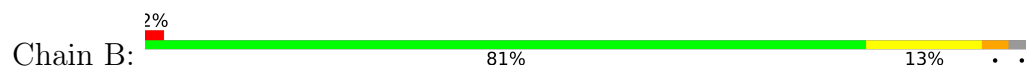


• Molecule 1: Polyprotein





• Molecule 2: Polyprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.94Å 102.07Å 251.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.78 50.00 – 2.78	Depositor EDS
% Data completeness (in resolution range)	92.2 (50.00-2.78) 92.2 (50.00-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0049, REFMAC 5.8.0049	Depositor
R, R_{free}	0.207 , 0.268 0.211 , 0.268	Depositor DCC
R_{free} test set	3119 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 13.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.069 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16942	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.77% 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

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

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	0.73	0/4313	0.97	3/5852 (0.1%)
1	C	0.77	1/4321 (0.0%)	0.97	6/5864 (0.1%)
1	D	0.75	0/4326	0.98	8/5871 (0.1%)
2	B	0.73	0/4323	0.99	10/5865 (0.2%)
All	All	0.74	1/17283 (0.0%)	0.98	27/23452 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	93	PRO	CA-C	6.12	1.55	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	352	ASP	CA-C-N	-10.93	111.79	119.66
2	B	352	ASP	C-N-CA	-10.93	111.79	119.66
1	A	352	ASP	CA-C-N	-8.07	112.07	120.38
1	A	352	ASP	C-N-CA	-8.07	112.07	120.38
1	D	352	ASP	CA-C-N	-7.25	114.44	119.66
1	D	352	ASP	C-N-CA	-7.25	114.44	119.66
1	A	201	VAL	CB-CA-C	-6.71	102.95	112.22
1	D	475	HIS	CA-C-N	-6.34	113.49	123.12
1	D	475	HIS	C-N-CA	-6.34	113.49	123.12
1	C	321	VAL	CB-CA-C	-5.88	101.93	110.63
2	B	490	ARG	N-CA-C	-5.78	104.90	111.14
2	B	390	THR	CA-C-N	-5.65	113.07	119.28
2	B	390	THR	C-N-CA	-5.65	113.07	119.28
2	B	539	ILE	N-CA-C	-5.50	103.56	108.95
2	B	304	ARG	N-CA-C	5.47	116.92	111.07
1	C	410	GLY	N-CA-C	-5.46	106.17	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	78	VAL	CB-CA-C	-5.37	104.26	110.91
1	C	475	HIS	CA-C-N	-5.34	114.55	123.04
1	C	475	HIS	C-N-CA	-5.34	114.55	123.04
1	D	201	VAL	CB-CA-C	-5.32	104.88	112.22
2	B	475	HIS	CA-C-N	-5.23	116.02	123.03
2	B	475	HIS	C-N-CA	-5.23	116.02	123.03
1	C	336	LEU	N-CA-C	5.21	116.65	111.07
1	D	258	GLU	N-CA-C	5.13	116.87	111.28
2	B	475	HIS	N-CA-C	5.13	121.72	110.80
1	D	275	GLY	N-CA-C	5.13	117.11	110.45
1	C	475	HIS	N-CA-C	5.04	121.54	110.80

There are no chirality outliers.

There are no planarity outliers.

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	4222	0	4212	45	0
1	C	4229	0	4219	47	0
1	D	4234	0	4224	56	0
2	B	4233	0	4228	47	0
3	A	12	0	8	2	0
3	B	12	0	8	1	0
All	All	16942	0	16899	195	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 (195) 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:253:ILE:O	1:C:257:THR:HG23	1.63	0.96
2:B:49:GLN:O	2:B:53:THR:HG23	1.68	0.92
1:A:49:GLN:O	1:A:53:THR:HG22	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:GLN:O	2:B:53:THR:CG2	2.23	0.86
1:A:237:GLU:HG3	1:A:257:THR:HG21	1.59	0.84
1:A:201:VAL:HG22	1:A:384:LEU:HD13	1.60	0.83
1:D:49:GLN:O	1:D:53:THR:HG22	1.79	0.81
1:D:203:PHE:O	1:D:207:THR:HG23	1.84	0.77
2:B:203:PHE:O	2:B:207:THR:HG23	1.84	0.76
1:D:49:GLN:O	1:D:53:THR:CG2	2.33	0.76
1:C:49:GLN:O	1:C:53:THR:CG2	2.34	0.75
2:B:201:VAL:HG22	2:B:384:LEU:HD13	1.70	0.74
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.70	0.74
1:D:196:SER:H	1:D:199:GLN:HE21	1.34	0.73
2:B:234:ARG:HG3	2:B:262:ILE:HD11	1.70	0.73
1:A:203:PHE:O	1:A:207:THR:HG23	1.90	0.72
1:C:237:GLU:HG3	1:C:257:THR:HG21	1.71	0.71
1:A:92:THR:O	1:A:109:ARG:NH1	2.23	0.71
2:B:396:ALA:O	2:B:399:THR:HG22	1.91	0.70
1:D:82:LEU:HD13	1:D:249:ALA:HB2	1.74	0.69
1:D:187:MET:HE1	1:D:292:THR:HG22	1.75	0.69
2:B:82:LEU:HD13	2:B:249:ALA:HB2	1.75	0.69
1:C:48:ARG:HG2	1:C:159:LEU:HD13	1.74	0.68
2:B:489:LEU:HA	2:B:494:VAL:HG13	1.77	0.67
2:B:33:HIS:HD2	2:B:491:LYS:O	1.78	0.67
1:C:203:PHE:O	1:C:207:THR:HG23	1.95	0.66
1:A:253:ILE:O	1:A:257:THR:HG23	1.96	0.65
1:C:489:LEU:HA	1:C:494:VAL:HG13	1.78	0.64
2:B:237:GLU:HG3	2:B:257:THR:HG21	1.81	0.63
1:C:6:TRP:HE1	1:C:53:THR:HG21	1.64	0.62
1:D:237:GLU:CG	1:D:257:THR:HG21	2.30	0.61
1:D:253:ILE:O	1:D:257:THR:HG23	2.00	0.61
1:C:49:GLN:O	1:C:53:THR:HG22	1.99	0.61
1:C:395:ALA:O	1:C:399:THR:HG22	2.01	0.61
1:C:187:MET:HE1	1:C:292:THR:HG22	1.82	0.61
1:D:187:MET:HE2	1:D:293:LEU:HD23	1.82	0.61
1:D:48:ARG:HG3	1:D:159:LEU:HD22	1.84	0.60
1:D:3:SER:OG	1:D:53:THR:HA	2.02	0.59
1:A:430:PHE:O	1:A:434:LEU:HB2	2.02	0.59
1:C:321:VAL:CG2	1:C:365:SER:CB	2.81	0.58
1:A:1:SER:OG	1:A:230:GLU:OE1	2.19	0.58
2:B:147:VAL:HG12	2:B:148:GLN:HG2	1.85	0.58
2:B:217:PHE:CD1	2:B:336:LEU:HD21	2.39	0.58
1:A:197:PRO:HG3	1:A:414:MET:HE3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ALA:HB3	1:D:245:LEU:CD2	2.34	0.57
1:A:530:VAL:O	1:A:531:LYS:CB	2.53	0.55
1:C:485:VAL:O	1:C:489:LEU:HG	2.06	0.55
2:B:448:TYR:CE2	2:B:551:PHE:HD1	2.25	0.54
2:B:489:LEU:HA	2:B:494:VAL:CG1	2.37	0.54
1:C:48:ARG:CG	1:C:159:LEU:HD13	2.38	0.54
1:A:419:LEU:HD23	1:A:485:VAL:HG21	1.90	0.54
1:C:187:MET:HE1	1:C:292:THR:CG2	2.37	0.54
1:C:1:SER:OG	1:C:230:GLU:OE1	2.25	0.54
1:D:201:VAL:HG22	1:D:384:LEU:HD13	1.90	0.53
1:A:170:CYS:HA	1:A:173:MET:HE3	1.90	0.53
2:B:419:LEU:HD13	2:B:477:TYR:CD2	2.43	0.53
1:C:527:ASN:O	1:C:530:VAL:HG23	2.09	0.53
1:C:340:THR:HG23	1:C:350:PRO:HG3	1.90	0.53
2:B:253:ILE:O	2:B:257:THR:HG23	2.09	0.53
1:C:49:GLN:O	1:C:53:THR:HG23	2.05	0.53
1:C:54:PHE:CD1	1:C:55:ASP:O	2.62	0.53
1:D:187:MET:HE2	1:D:293:LEU:CD2	2.38	0.53
1:A:414:MET:HE2	3:A:601:3AV:H6	1.91	0.53
2:B:217:PHE:CE1	2:B:336:LEU:HD21	2.45	0.52
1:D:530:VAL:O	1:D:531:LYS:HB2	2.10	0.52
2:B:6:TRP:HE1	2:B:53:THR:HG21	1.75	0.52
1:C:203:PHE:O	1:C:207:THR:CG2	2.57	0.52
1:A:414:MET:HE1	1:A:551:PHE:CE1	2.45	0.51
1:D:6:TRP:HE1	1:D:53:THR:HG21	1.74	0.51
2:B:200:ARG:HD2	3:B:601:3AV:H1	1.92	0.50
1:D:448:TYR:CE2	1:D:551:PHE:HD1	2.29	0.50
1:A:31:LEU:HD12	1:A:31:LEU:O	2.11	0.50
2:B:306:ALA:HB3	2:B:308:LEU:HD22	1.93	0.50
1:C:82:LEU:HD13	1:C:249:ALA:HB2	1.93	0.50
1:D:530:VAL:O	1:D:531:LYS:CB	2.60	0.50
1:D:48:ARG:CG	1:D:159:LEU:HD22	2.41	0.49
2:B:237:GLU:CG	2:B:257:THR:HG21	2.41	0.49
2:B:196:SER:H	2:B:199:GLN:HE21	1.61	0.49
1:C:182:LEU:HD13	1:C:243:CYS:SG	2.53	0.49
1:A:253:ILE:O	1:A:257:THR:CG2	2.61	0.49
1:C:387:ASP:OD2	1:C:387:ASP:C	2.56	0.49
1:D:419:LEU:HD13	1:D:477:TYR:CD2	2.47	0.49
1:D:396:ALA:O	1:D:399:THR:HG22	2.13	0.49
1:A:508:ARG:HG3	1:A:526:PHE:HB2	1.95	0.48
1:C:433:LEU:HB3	1:C:439:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508:ARG:HG3	1:D:526:PHE:HB2	1.95	0.48
1:C:321:VAL:CG2	1:C:365:SER:HB3	2.43	0.48
1:D:231:ASN:O	1:D:235:VAL:HG23	2.14	0.48
1:C:434:LEU:HD21	1:C:510:ARG:HB2	1.96	0.47
1:A:241:GLN:OE1	1:A:250:ARG:HG3	2.14	0.47
1:D:306:ALA:HB3	1:D:308:LEU:HD22	1.94	0.47
2:B:48:ARG:HG2	2:B:159:LEU:HD13	1.95	0.47
2:B:489:LEU:CA	2:B:494:VAL:HG13	2.44	0.47
2:B:321:VAL:CG2	2:B:365:SER:CB	2.93	0.47
1:C:197:PRO:O	1:C:201:VAL:HG23	2.14	0.47
2:B:105:ALA:O	2:B:109:ARG:HG3	2.14	0.47
1:A:385:THR:OG1	1:A:386:ARG:N	2.47	0.47
1:D:80:ALA:HB3	1:D:245:LEU:HD21	1.97	0.46
1:A:61:ASP:O	1:A:65:ARG:HG3	2.15	0.46
2:B:49:GLN:O	2:B:53:THR:HG22	2.14	0.46
1:D:281:ALA:O	1:D:287:THR:OG1	2.31	0.46
1:D:314:LEU:HB3	1:D:321:VAL:HG23	1.96	0.46
1:D:182:LEU:HD13	1:D:243:CYS:SG	2.56	0.46
1:A:213:ASN:ND2	1:A:326:SER:HB3	2.31	0.46
1:A:241:GLN:OE1	1:A:250:ARG:CG	2.64	0.46
2:B:196:SER:H	2:B:199:GLN:NE2	2.13	0.46
1:C:530:VAL:O	1:C:531:LYS:CB	2.64	0.45
1:C:555:TYR:O	1:C:556:SER:C	2.59	0.45
1:D:80:ALA:HB3	1:D:245:LEU:HD23	1.98	0.45
1:A:489:LEU:HA	1:A:494:VAL:HG13	1.99	0.45
1:C:523:LYS:HG3	1:C:534:LEU:HD12	1.99	0.45
2:B:200:ARG:HD3	2:B:384:LEU:HD21	1.98	0.45
2:B:237:GLU:HG3	2:B:257:THR:CG2	2.45	0.45
1:C:321:VAL:HG22	1:C:365:SER:HB3	1.99	0.45
1:A:3:SER:OG	1:A:53:THR:HA	2.16	0.45
2:B:40:THR:HB	2:B:157:ALA:HB2	1.98	0.45
2:B:336:LEU:HD12	2:B:356:PRO:HG3	1.99	0.45
1:D:187:MET:CE	1:D:292:THR:HG22	2.46	0.45
1:D:119:ILE:HD13	1:D:169:VAL:HG11	1.99	0.45
1:D:11:ILE:HD12	1:D:45:ALA:HB1	1.98	0.45
1:C:22:PRO:HD2	1:C:400:ALA:HB1	1.99	0.44
1:A:48:ARG:HG2	1:A:159:LEU:HD13	2.00	0.44
2:B:530:VAL:O	2:B:531:LYS:CB	2.65	0.44
1:D:146:CYS:SG	1:D:147:VAL:N	2.91	0.44
1:D:230:GLU:O	1:D:234:ARG:HG3	2.17	0.44
1:D:314:LEU:HD12	1:D:314:LEU:HA	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:GLU:O	1:C:238:SER:C	2.60	0.44
1:A:212:LYS:N	1:A:325:GLU:OE1	2.50	0.44
1:C:196:SER:H	1:C:199:GLN:HE21	1.63	0.44
1:C:434:LEU:HD21	1:C:510:ARG:CB	2.48	0.43
1:A:167:VAL:O	1:A:168:ARG:C	2.61	0.43
1:C:3:SER:OG	1:C:53:THR:HA	2.17	0.43
1:C:72:LYS:HG2	1:C:242:CYS:SG	2.57	0.43
2:B:445:CYS:SG	2:B:454:ILE:HD12	2.59	0.43
1:D:200:ARG:HD3	1:D:384:LEU:HD21	2.01	0.43
1:D:445:CYS:SG	1:D:454:ILE:HD12	2.58	0.43
1:A:40:THR:HB	1:A:157:ALA:HB2	2.00	0.43
1:D:263:GLY:HA2	1:D:277:ARG:NH1	2.34	0.43
1:A:233:ILE:CG2	1:A:262:ILE:HD12	2.48	0.43
1:C:54:PHE:HD1	1:C:55:ASP:O	1.99	0.43
1:D:196:SER:OG	1:D:199:GLN:HG3	2.17	0.43
2:B:385:THR:OG1	2:B:386:ARG:N	2.52	0.43
1:D:489:LEU:HA	1:D:494:VAL:HG13	2.01	0.43
1:A:408:TRP:HE3	1:A:412:ILE:HD12	1.84	0.43
1:D:129:ASP:O	1:D:259:ARG:HD2	2.19	0.43
1:A:219:TYR:HB3	1:A:320:LEU:HD23	2.01	0.42
1:A:321:VAL:HG22	1:A:365:SER:CB	2.48	0.42
1:A:408:TRP:CE3	1:A:412:ILE:HD12	2.54	0.42
1:D:445:CYS:SG	1:D:454:ILE:CD1	3.07	0.42
2:B:321:VAL:CG2	2:B:365:SER:HB2	2.49	0.42
1:D:33:HIS:HD2	1:D:491:LYS:O	2.02	0.42
1:A:216:GLY:HA2	1:A:322:VAL:O	2.18	0.42
1:A:374:HIS:HA	1:A:379:LYS:O	2.20	0.42
1:A:527:ASN:HD21	1:A:533:LYS:HB3	1.84	0.42
2:B:201:VAL:O	2:B:205:VAL:HG23	2.18	0.42
1:D:49:GLN:O	1:D:53:THR:HG23	2.17	0.42
2:B:17:GLU:OE1	2:B:42:SER:OG	2.38	0.42
1:A:182:LEU:N	1:A:183:PRO:CD	2.83	0.42
1:A:423:MET:HA	1:A:528:TRP:CZ2	2.55	0.42
1:C:21:LEU:HD22	1:C:37:VAL:HB	2.02	0.42
1:C:5:THR:HG23	1:C:278:ARG:NH2	2.34	0.42
2:B:537:THR:O	2:B:538:PRO:C	2.61	0.41
1:C:175:LEU:HD13	1:C:286:THR:CG2	2.49	0.41
1:D:481:GLU:O	1:D:485:VAL:HG23	2.20	0.41
1:A:5:THR:O	1:A:275:GLY:HA3	2.20	0.41
1:A:200:ARG:HD3	1:A:384:LEU:HD21	2.02	0.41
1:A:436:GLN:O	1:A:437:GLU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:PRO:HG3	1:C:289:CYS:SG	2.61	0.41
1:C:385:THR:OG1	1:C:386:ARG:N	2.52	0.41
1:A:237:GLU:OE2	1:A:254:LYS:HD2	2.19	0.41
1:D:422:ARG:NH2	1:D:528:TRP:HB3	2.35	0.41
2:B:321:VAL:HG22	2:B:365:SER:CB	2.51	0.41
1:C:211:LYS:HB2	1:C:214:PRO:HB3	2.02	0.41
1:A:366:CYS:O	3:A:601:3AV:H4	2.20	0.41
1:D:309:GLN:O	1:D:310:ASP:C	2.63	0.41
1:D:559:ASP:C	1:D:560:ILE:HG12	2.46	0.41
2:B:21:LEU:CD2	2:B:37:VAL:HB	2.51	0.41
2:B:416:ALA:N	2:B:417:PRO:CD	2.84	0.41
1:D:104:GLY:N	1:D:107:ASP:OD2	2.47	0.41
1:D:215:MET:HE2	1:D:332:ASP:HB3	2.02	0.41
1:A:28:ASN:O	1:A:28:ASN:ND2	2.54	0.40
2:B:106:LYS:CD	2:B:106:LYS:H	2.34	0.40
2:B:233:ILE:HD13	2:B:261:TYR:O	2.21	0.40
2:B:434:LEU:HD13	2:B:439:LEU:HD11	2.02	0.40
1:D:187:MET:HE1	1:D:292:THR:CG2	2.46	0.40
1:D:423:MET:HA	1:D:528:TRP:CZ2	2.56	0.40
1:D:470:SER:O	1:D:474:LEU:HG	2.21	0.40
2:B:422:ARG:HA	2:B:426:MET:SD	2.61	0.40
1:C:253:ILE:O	1:C:257:THR:CG2	2.52	0.40
1:C:407:SER:O	1:C:408:TRP:C	2.63	0.40
1:D:336:LEU:HD12	1:D:354:PRO:HB2	2.04	0.40
1:C:12:THR:OG1	1:C:269:SER:OG	2.16	0.40
1:D:113:SER:O	1:D:117:ASN:HB3	2.21	0.40
1:D:203:PHE:CE2	1:D:314:LEU:HD13	2.56	0.40
2:B:30:LEU:HD12	2:B:30:LEU:HA	1.91	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%)	502 (94%)	32 (6%)	2 (0%)	30	57
1	C	537/566 (95%)	505 (94%)	30 (6%)	2 (0%)	30	57
1	D	538/566 (95%)	504 (94%)	31 (6%)	3 (1%)	21	47
2	B	539/566 (95%)	511 (95%)	27 (5%)	1 (0%)	43	70
All	All	2150/2264 (95%)	2022 (94%)	120 (6%)	8 (0%)	30	57

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	531	LYS
2	B	531	LYS
1	C	531	LYS
1	D	531	LYS
1	D	367	SER
1	D	540	PRO
1	C	400	ALA
1	A	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%)	421 (92%)	39 (8%)	10	28
1	C	461/482 (96%)	432 (94%)	29 (6%)	16	41
1	D	461/482 (96%)	427 (93%)	34 (7%)	13	34
2	B	461/482 (96%)	429 (93%)	32 (7%)	14	38
All	All	1843/1928 (96%)	1709 (93%)	134 (7%)	13	35

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	29	SER
1	A	34	HIS

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Mol	Chain	Res	Type
1	A	51	LYS
1	A	76	SER
1	A	79	LYS
1	A	82	LEU
1	A	100	LYS
1	A	106	LYS
1	A	113	SER
1	A	139	MET
1	A	148	GLN
1	A	159	LEU
1	A	160	ILE
1	A	184	GLN
1	A	190	SER
1	A	201	VAL
1	A	207	THR
1	A	222	ARG
1	A	230	GLU
1	A	254	LYS
1	A	257	THR
1	A	262	ILE
1	A	308	LEU
1	A	315	VAL
1	A	321	VAL
1	A	330	GLN
1	A	336	LEU
1	A	352	ASP
1	A	368	SER
1	A	384	LEU
1	A	403	THR
1	A	434	LEU
1	A	437	GLU
1	A	473	SER
1	A	478	SER
1	A	494	VAL
1	A	539	ILE
1	A	556	SER
2	B	14	CYS
2	B	21	LEU
2	B	42	SER
2	B	53	THR
2	B	82	LEU
2	B	83	LEU

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Mol	Chain	Res	Type
2	B	90	LYS
2	B	106	LYS
2	B	112	SER
2	B	128	GLU
2	B	159	LEU
2	B	160	ILE
2	B	207	THR
2	B	222	ARG
2	B	230	GLU
2	B	257	THR
2	B	262	ILE
2	B	308	LEU
2	B	315	VAL
2	B	321	VAL
2	B	329	THR
2	B	330	GLN
2	B	335	SER
2	B	405	VAL
2	B	434	LEU
2	B	440	GLU
2	B	492	LEU
2	B	494	VAL
2	B	530	VAL
2	B	532	THR
2	B	548	SER
2	B	556	SER
1	C	14	CYS
1	C	21	LEU
1	C	50	LYS
1	C	53	THR
1	C	82	LEU
1	C	100	LYS
1	C	106	LYS
1	C	147	VAL
1	C	159	LEU
1	C	184	GLN
1	C	207	THR
1	C	222	ARG
1	C	230	GLU
1	C	254	LYS
1	C	257	THR
1	C	262	ILE

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Mol	Chain	Res	Type
1	C	308	LEU
1	C	330	GLN
1	C	336	LEU
1	C	367	SER
1	C	380	ARG
1	C	387	ASP
1	C	398	GLU
1	C	399	THR
1	C	405	VAL
1	C	464	GLU
1	C	494	VAL
1	C	513	SER
1	C	530	VAL
1	D	53	THR
1	D	74	LYS
1	D	106	LYS
1	D	113	SER
1	D	117	ASN
1	D	135	ASP
1	D	147	VAL
1	D	159	LEU
1	D	184	GLN
1	D	222	ARG
1	D	230	GLU
1	D	257	THR
1	D	262	ILE
1	D	308	LEU
1	D	313	MET
1	D	315	VAL
1	D	321	VAL
1	D	330	GLN
1	D	336	LEU
1	D	368	SER
1	D	369	ASN
1	D	380	ARG
1	D	384	LEU
1	D	394	ARG
1	D	405	VAL
1	D	431	SER
1	D	434	LEU
1	D	441	LYS
1	D	469	LEU

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Mol	Chain	Res	Type
1	D	494	VAL
1	D	530	VAL
1	D	552	VAL
1	D	556	SER
1	D	560	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	120	HIS
1	A	142	ASN
1	A	199	GLN
1	A	213	ASN
1	A	428	HIS
1	A	527	ASN
2	B	33	HIS
2	B	58	GLN
2	B	199	GLN
2	B	273	ASN
2	B	428	HIS
1	C	28	ASN
1	C	58	GLN
1	C	63	HIS
1	C	184	GLN
1	C	199	GLN
1	C	273	ASN
1	C	411	ASN
1	C	436	GLN
1	C	562	HIS
1	D	28	ASN
1	D	33	HIS
1	D	58	GLN
1	D	199	GLN
1	D	502	HIS
1	D	562	HIS

5.3.3 RNA ⓘ

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](#)

2 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
3	3AV	B	601	-	13,13,13	2.35	2 (15%)	18,18,18	1.47	3 (16%)
3	3AV	A	601	-	13,13,13	2.29	1 (7%)	18,18,18	1.45	4 (22%)

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	3AV	B	601	-	-	-	0/2/2/2
3	3AV	A	601	-	-	-	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	3AV	O-C04	7.50	1.36	1.21
3	A	601	3AV	O-C04	7.36	1.36	1.21
3	B	601	3AV	C07-C05	2.25	1.38	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	601	3AV	O01-C02-C09	2.82	123.68	120.51
3	B	601	3AV	C09-C05-C07	-2.69	117.78	121.52
3	B	601	3AV	O01-C02-C09	2.61	123.44	120.51
3	A	601	3AV	C09-C05-C07	-2.35	118.25	121.52
3	A	601	3AV	C02-O01-C04	-2.32	118.78	121.67
3	B	601	3AV	C02-O01-C04	-2.13	119.02	121.67
3	A	601	3AV	C03-C-C08	-2.09	118.96	121.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	3AV	1	0
3	A	601	3AV	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	544/566 (96%)	0.05	11 (2%) 65 58	16, 30, 50, 71	0
1	C	545/566 (96%)	-0.03	8 (1%) 72 65	17, 30, 47, 71	0
1	D	546/566 (96%)	0.04	14 (2%) 57 49	18, 30, 52, 81	0
2	B	547/566 (96%)	-0.02	14 (2%) 57 49	18, 29, 48, 91	0
All	All	2182/2264 (96%)	0.01	47 (2%) 62 55	16, 30, 50, 91	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	541	ALA	5.9
2	B	542	ALA	5.3
2	B	549	GLY	4.1
1	C	548	SER	3.8
2	B	404	PRO	3.8
1	A	539	ILE	3.7
1	C	549	GLY	3.6
1	A	148	GLN	3.6
1	D	28	ASN	3.5
1	C	29	SER	3.4
1	D	548	SER	3.4
2	B	405	VAL	3.4
1	D	549	GLY	3.3
1	D	148	GLN	3.2
1	A	22	PRO	3.1
1	A	562	HIS	3.1
1	D	540	PRO	3.1
1	D	120	HIS	2.9
2	B	376	ALA	2.9
2	B	530	VAL	2.8
1	D	262	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	549	GLY	2.7
1	C	402	HIS	2.7
1	A	548	SER	2.6
1	D	29	SER	2.6
2	B	29	SER	2.5
1	A	405	VAL	2.5
2	B	148	GLN	2.5
1	C	148	GLN	2.5
2	B	548	SER	2.5
1	D	404	PRO	2.5
1	C	405	VAL	2.4
1	D	402	HIS	2.3
1	D	530	VAL	2.3
2	B	541	ALA	2.2
1	D	22	PRO	2.2
2	B	22	PRO	2.2
2	B	540	PRO	2.2
1	A	29	SER	2.2
2	B	562	HIS	2.2
1	A	530	VAL	2.1
1	D	403	THR	2.1
1	A	254	LYS	2.1
1	A	404	PRO	2.1
1	C	22	PRO	2.1
2	B	402	HIS	2.1
1	C	262	ILE	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 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
3	3AV	A	601	12/12	0.81	0.22	57,63,66,68	0
3	3AV	B	601	12/12	0.86	0.21	69,73,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.