



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:48 AM EDT

PDB ID : 3Q6M / pdb_00003q6m
Title : Crystal Structure of Human MC-HSP90 in C2221 Space Group
Authors : Lee, C.C.; Lin, T.W.; Ko, T.P.; Wang, A.H.-J.
Deposited on : 2011-01-03
Resolution : 3.00 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

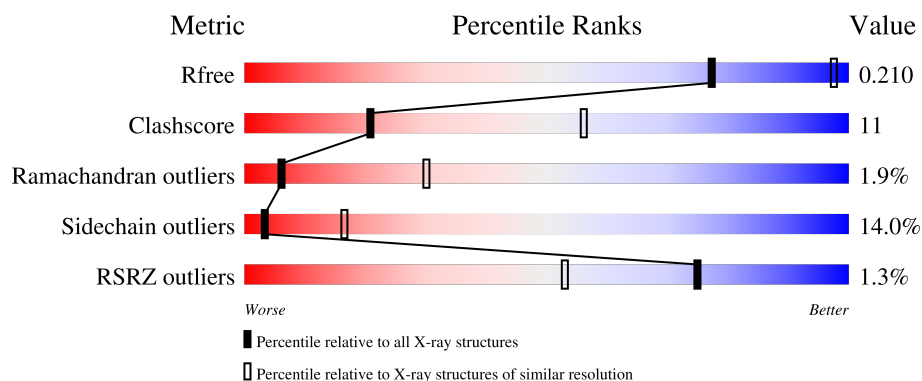
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	448	
1	B	448	
1	C	448	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9345 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 Heat shock protein HSP 90-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			3069	1954	518	582	15			
1	B	374	Total	C	N	O	S	0	0	0
			3085	1964	520	586	15			
1	C	369	Total	C	N	O	S	0	0	0
			3043	1939	512	577	15			

There are 24 discrepancies between the modelled and reference sequences:

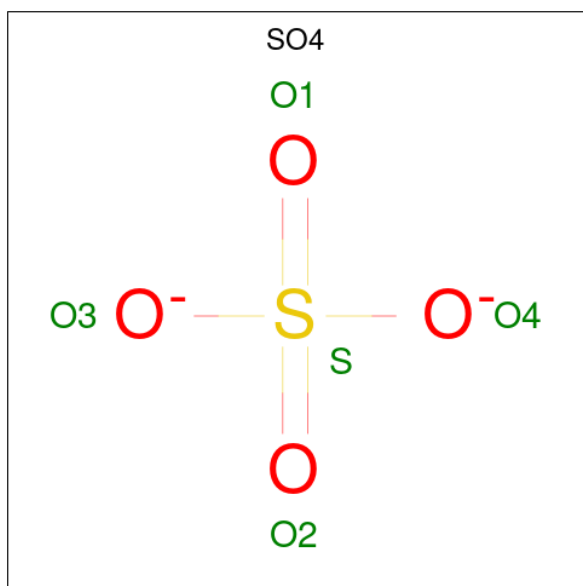
Chain	Residue	Modelled	Actual	Comment	Reference
A	291	ALA	-	expression tag	UNP P07900
A	292	ALA	-	expression tag	UNP P07900
A	733	HIS	-	expression tag	UNP P07900
A	734	HIS	-	expression tag	UNP P07900
A	735	HIS	-	expression tag	UNP P07900
A	736	HIS	-	expression tag	UNP P07900
A	737	HIS	-	expression tag	UNP P07900
A	738	HIS	-	expression tag	UNP P07900
B	291	ALA	-	expression tag	UNP P07900
B	292	ALA	-	expression tag	UNP P07900
B	733	HIS	-	expression tag	UNP P07900
B	734	HIS	-	expression tag	UNP P07900
B	735	HIS	-	expression tag	UNP P07900
B	736	HIS	-	expression tag	UNP P07900
B	737	HIS	-	expression tag	UNP P07900
B	738	HIS	-	expression tag	UNP P07900
C	291	ALA	-	expression tag	UNP P07900
C	292	ALA	-	expression tag	UNP P07900
C	733	HIS	-	expression tag	UNP P07900
C	734	HIS	-	expression tag	UNP P07900
C	735	HIS	-	expression tag	UNP P07900
C	736	HIS	-	expression tag	UNP P07900
C	737	HIS	-	expression tag	UNP P07900

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Chain	Residue	Modelled	Actual	Comment	Reference
C	738	HIS	-	expression tag	UNP P07900

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

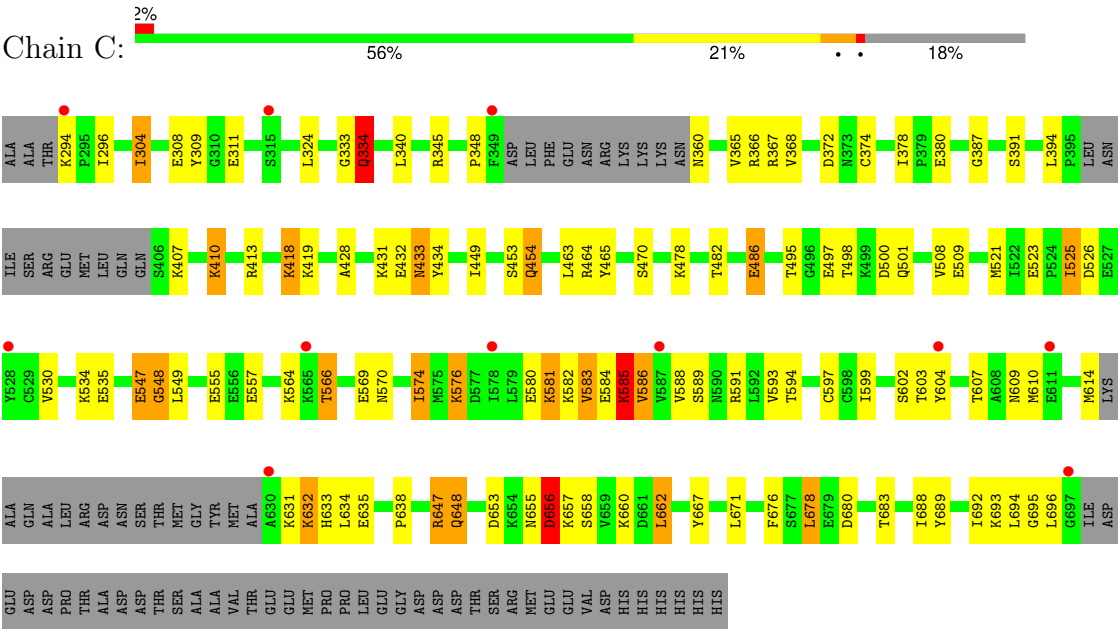


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	53	Total	O	0	0
			53	53		
3	C	36	Total	O	0	0
			36	36		

● Molecule 1: Heat shock protein HSP 90-alpha



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	162.70Å 304.55Å 87.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-3.00) 94.9 (30.00-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 3.00Å)	Xtriage
Refinement program	CNS 1.2, REFMAC 5.5.0109	Depositor
R, R_{free}	0.209 , 0.252 0.211 , 0.210	Depositor DCC
R_{free} test set	2184 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	88.1	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 83.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9345	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: SO4

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	0.71	0/3120	0.97	3/4188 (0.1%)
1	B	0.74	0/3136	0.99	4/4210 (0.1%)
1	C	0.66	0/3094	0.94	6/4154 (0.1%)
All	All	0.70	0/9350	0.96	13/12552 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	THR	N-CA-C	6.51	119.55	109.60
1	B	433	ASN	N-CA-C	5.95	120.49	113.23
1	A	294	LYS	CA-C-N	-5.93	114.50	120.31
1	A	294	LYS	C-N-CA	-5.93	114.50	120.31
1	C	387	GLY	N-CA-C	5.82	118.02	110.45
1	B	438	TYR	N-CA-C	5.75	117.55	111.28
1	C	294	LYS	CA-C-N	-5.34	114.74	120.03
1	C	294	LYS	C-N-CA	-5.34	114.74	120.03
1	B	431	LYS	N-CA-C	5.17	117.81	111.82
1	C	311	GLU	N-CA-C	-5.07	105.03	111.11
1	C	695	GLY	N-CA-C	-5.06	107.77	115.66
1	B	434	TYR	N-CA-C	-5.04	105.88	112.23
1	C	470	SER	N-CA-C	5.02	120.03	113.30

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	3069	0	3108	74	0
1	B	3085	0	3123	73	0
1	C	3043	0	3081	67	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	44	0	0	1	0
3	B	53	0	0	0	0
3	C	36	0	0	1	0
All	All	9345	0	9312	205	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 11.

All (205) 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:B:367:ARG:HH11	1:B:367:ARG:HG3	1.15	1.03
1:A:691:MET:SD	1:B:691:MET:HE3	2.02	1.00
1:C:607:THR:HG22	1:C:610:MET:HG3	1.43	0.99
1:B:410:LYS:HE3	1:B:414:LYS:HE3	1.44	0.97
1:C:525:ILE:HD12	1:C:525:ILE:H	1.32	0.94
1:A:656:ASP:HB3	1:A:659:VAL:HG23	1.48	0.93
1:A:525:ILE:HD12	1:A:525:ILE:H	1.35	0.91
1:B:525:ILE:H	1:B:525:ILE:HD12	1.38	0.89
1:A:680:ASP:OD2	1:A:683:THR:HG23	1.73	0.87
1:C:576:LYS:HB3	1:C:586:VAL:HG12	1.58	0.86
1:C:589:SER:HB2	1:C:635:GLU:HB3	1.56	0.85
1:B:655:ASN:H	1:B:655:ASN:HD22	1.21	0.84
1:B:367:ARG:HH11	1:B:367:ARG:CG	1.93	0.82
1:C:647:ARG:HH11	1:C:647:ARG:HG2	1.47	0.79
1:B:509:GLU:HB3	1:B:593:VAL:HG22	1.65	0.78
1:A:486:GLU:OE2	1:A:486:GLU:HA	1.85	0.77
1:A:429:GLU:O	1:A:430:ASP:C	2.28	0.76
1:A:509:GLU:HB3	1:A:593:VAL:HG13	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:LYS:HE3	1:B:414:LYS:CE	2.16	0.76
1:B:410:LYS:CE	1:B:414:LYS:HE3	2.17	0.75
1:C:607:THR:H	1:C:610:MET:HE3	1.52	0.74
1:C:593:VAL:HG23	1:C:594:THR:HG23	1.69	0.74
1:B:606:TRP:HE3	1:B:630:ALA:N	1.86	0.74
1:B:296:ILE:HD11	1:B:304:ILE:HD13	1.69	0.74
1:B:346:ARG:HG3	1:B:346:ARG:HH11	1.52	0.74
1:B:655:ASN:H	1:B:655:ASN:ND2	1.87	0.71
1:B:641:SER:O	1:B:645:THR:HG23	1.90	0.71
1:C:688:ILE:O	1:C:692:ILE:HG22	1.91	0.71
1:C:304:ILE:HD12	1:C:308:GLU:HB2	1.73	0.71
1:A:688:ILE:O	1:A:692:ILE:HG23	1.91	0.70
1:C:525:ILE:H	1:C:525:ILE:CD1	2.03	0.70
1:B:660:LYS:HB3	1:B:660:LYS:NZ	2.06	0.70
1:A:443:LYS:HG3	1:A:525:ILE:HG12	1.72	0.69
1:B:414:LYS:NZ	1:B:454:GLN:HE22	1.90	0.69
1:B:655:ASN:HD22	1:B:655:ASN:N	1.85	0.69
1:C:564:LYS:HG2	1:C:638:PRO:HB3	1.76	0.68
1:B:392:GLU:O	1:B:393:ASP:HB2	1.94	0.68
1:A:366:ARG:NH1	1:A:393:ASP:HA	2.09	0.68
1:A:614:MET:O	1:A:614:MET:HG3	1.94	0.68
1:C:580:GLU:O	1:C:581:LYS:HB3	1.94	0.68
1:C:431:LYS:O	1:C:433:ASN:N	2.26	0.67
1:B:367:ARG:HG3	1:B:367:ARG:NH1	1.93	0.67
1:C:607:THR:N	1:C:610:MET:HE3	2.10	0.67
1:C:431:LYS:C	1:C:433:ASN:H	2.02	0.67
1:C:296:ILE:HD11	1:C:304:ILE:HD13	1.78	0.66
1:A:656:ASP:HB3	1:A:659:VAL:CG2	2.26	0.65
1:B:578:ILE:HG21	1:B:660:LYS:HG2	1.79	0.63
1:C:410:LYS:NZ	1:C:413:ARG:HD3	2.13	0.63
1:C:564:LYS:HG2	1:C:638:PRO:CB	2.30	0.62
1:C:304:ILE:HG12	1:C:309:TYR:CZ	2.35	0.61
1:B:698:ILE:O	1:B:699:ASP:CB	2.48	0.61
1:A:692:ILE:HD12	1:B:662:LEU:HD11	1.82	0.60
1:B:509:GLU:OE2	1:B:595:SER:HB2	2.00	0.60
1:B:578:ILE:HD12	1:B:660:LYS:HA	1.84	0.60
1:C:583:VAL:HG22	1:C:632:LYS:HB2	1.84	0.60
1:B:405:GLN:HG3	1:B:406:SER:N	2.16	0.59
1:C:647:ARG:HH12	1:C:648:GLN:HG3	1.67	0.59
1:B:304:ILE:HG12	1:B:309:TYR:CZ	2.36	0.59
1:C:566:THR:HA	1:C:569:GLU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:ILE:O	1:B:699:ASP:HB3	2.02	0.59
1:C:570:ASN:O	1:C:574:ILE:HG23	2.03	0.59
1:A:466:TYR:CE2	1:A:474:MET:HE2	2.37	0.58
1:A:691:MET:HG2	1:B:691:MET:SD	2.43	0.58
1:A:526:ASP:O	1:A:530:VAL:HG22	2.03	0.57
1:C:449:ILE:HD13	1:C:463:LEU:HD11	1.86	0.57
1:A:338:ARG:HH11	1:A:338:ARG:HB2	1.68	0.57
1:A:662:LEU:HD11	1:B:692:ILE:HD12	1.85	0.57
1:C:367:ARG:N	1:C:367:ARG:HD3	2.20	0.57
1:B:463:LEU:O	1:B:464:ARG:HD3	2.04	0.56
1:A:679:GLU:H	1:A:679:GLU:CD	2.14	0.56
1:C:647:ARG:HG2	1:C:647:ARG:NH1	2.19	0.56
1:A:684:HIS:O	1:A:688:ILE:HG12	2.05	0.55
1:A:447:LEU:O	1:A:451:GLU:HG2	2.06	0.55
1:A:695:GLY:O	1:A:696:LEU:HD12	2.07	0.55
1:A:692:ILE:HD11	1:B:666:LEU:HD21	1.88	0.55
1:C:602:SER:HB2	1:C:631:LYS:HD2	1.87	0.55
1:C:418:LYS:HE2	1:C:419:LYS:HD3	1.88	0.54
1:A:536:PHE:CD2	1:A:537:GLU:HB2	2.43	0.54
1:A:566:THR:HA	1:A:569:GLU:HB2	1.89	0.54
1:C:582:LYS:HB3	1:C:667:TYR:CE2	2.43	0.54
1:A:307:GLU:H	1:A:307:GLU:CD	2.16	0.54
1:C:526:ASP:O	1:C:530:VAL:HG22	2.08	0.54
1:C:486:GLU:HA	1:C:486:GLU:OE1	2.06	0.54
1:C:689:TYR:HA	1:C:692:ILE:HG22	1.89	0.54
1:C:497:GLU:HG2	1:C:501:GLN:OE1	2.07	0.54
1:A:692:ILE:HG22	1:B:691:MET:SD	2.49	0.53
1:C:428:ALA:HA	1:C:434:TYR:CD1	2.44	0.53
1:B:497:GLU:H	1:B:501:GLN:HE22	1.57	0.53
1:A:578:ILE:HD11	1:A:664:ILE:HG13	1.91	0.52
1:B:304:ILE:HD12	1:B:308:GLU:CB	2.39	0.52
1:A:691:MET:SD	1:B:691:MET:CE	2.88	0.52
1:A:435:LYS:NZ	3:A:100:HOH:O	2.39	0.52
1:B:513:LYS:HD3	1:B:514:HIS:CE1	2.45	0.52
1:B:688:ILE:O	1:B:692:ILE:HG23	2.09	0.52
1:C:410:LYS:HZ2	1:C:413:ARG:HD3	1.75	0.52
1:A:480:TYR:CE2	1:A:517:GLU:HB3	2.45	0.51
1:A:362:LYS:HD3	1:A:372:ASP:HB3	1.92	0.51
1:B:660:LYS:HB3	1:B:660:LYS:HZ3	1.76	0.51
1:C:689:TYR:O	1:C:693:LYS:HB2	2.11	0.51
1:B:450:HIS:HD2	1:B:528:TYR:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:MET:O	1:B:614:MET:HG2	2.10	0.50
1:A:691:MET:O	1:A:694:LEU:HB3	2.11	0.50
1:A:602:SER:HB3	1:A:631:LYS:HB2	1.93	0.50
1:A:684:HIS:CE1	1:A:688:ILE:HD11	2.47	0.50
1:C:296:ILE:HD11	1:C:304:ILE:CD1	2.42	0.50
1:C:431:LYS:C	1:C:433:ASN:N	2.70	0.50
1:B:346:ARG:HG3	1:B:346:ARG:NH1	2.22	0.50
1:A:580:GLU:HG3	1:A:581:LYS:H	1.77	0.50
1:A:578:ILE:HD13	1:A:660:LYS:HG3	1.94	0.49
1:B:525:ILE:H	1:B:525:ILE:CD1	2.11	0.49
1:A:585:LYS:HG2	1:A:587:VAL:HG13	1.94	0.49
1:B:297:TRP:CD2	1:B:388:VAL:HG21	2.47	0.49
1:A:494:ILE:HB	1:A:544:VAL:HG22	1.94	0.49
1:C:680:ASP:O	1:C:683:THR:HG22	2.13	0.49
1:B:414:LYS:HZ3	1:B:454:GLN:HE22	1.60	0.49
1:B:604:TYR:H	1:B:604:TYR:HD2	1.58	0.49
1:C:593:VAL:HG23	1:C:594:THR:N	2.27	0.49
1:B:304:ILE:HD12	1:B:308:GLU:HB2	1.93	0.49
1:A:338:ARG:HB2	1:A:338:ARG:NH1	2.28	0.48
1:C:585:LYS:HG3	1:C:633:HIS:HD2	1.78	0.48
1:B:498:THR:O	1:B:502:VAL:HG22	2.13	0.48
1:C:366:ARG:NH1	3:C:122:HOH:O	2.46	0.48
1:B:578:ILE:C	1:B:580:GLU:H	2.21	0.48
1:C:689:TYR:HA	1:C:692:ILE:CG2	2.43	0.48
1:A:366:ARG:HH12	1:A:393:ASP:HA	1.79	0.48
1:C:547:GLU:HG3	1:C:548:GLY:N	2.27	0.48
1:C:324:LEU:HB2	1:C:345:ARG:HG2	1.95	0.47
1:B:566:THR:HA	1:B:569:GLU:HB2	1.96	0.47
1:A:604:TYR:HB3	1:A:631:LYS:NZ	2.29	0.47
1:C:365:VAL:HG22	1:C:391:SER:HB3	1.97	0.47
1:B:304:ILE:HG12	1:B:309:TYR:CE1	2.50	0.46
1:B:660:LYS:HB3	1:B:660:LYS:HZ2	1.80	0.46
1:B:490:HIS:HB3	1:B:542:VAL:CG1	2.45	0.46
1:A:554:ASP:OD2	1:A:556:GLU:HB3	2.15	0.46
1:B:495:THR:HA	1:B:521:MET:O	2.15	0.46
1:C:602:SER:HB2	1:C:633:HIS:HE1	1.80	0.46
1:A:582:LYS:HD2	1:A:667:TYR:CE2	2.50	0.46
1:A:642:ILE:O	1:A:646:LEU:HB2	2.15	0.46
1:C:607:THR:HG23	1:C:609:ASN:H	1.81	0.46
1:B:443:LYS:HG3	1:B:525:ILE:HG12	1.98	0.46
1:C:658:SER:O	1:C:662:LEU:HD22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:LEU:O	1:A:580:GLU:C	2.58	0.45
1:A:495:THR:HG22	1:A:521:MET:HB2	1.98	0.45
1:C:671:LEU:HG	1:C:676:PHE:HB2	1.98	0.45
1:A:535:GLU:HB3	1:A:540:THR:HA	1.98	0.45
1:A:579:LEU:HD11	1:A:667:TYR:HB2	1.98	0.45
1:A:364:TYR:HB3	1:A:390:ASP:OD2	2.17	0.45
1:A:688:ILE:HD12	1:B:688:ILE:HD12	1.99	0.44
1:A:450:HIS:HD2	1:A:451:GLU:OE1	2.00	0.44
1:C:333:GLY:O	1:C:334:GLN:C	2.61	0.44
1:A:525:ILE:H	1:A:525:ILE:CD1	2.08	0.44
1:B:527:GLU:HG2	1:B:610:MET:HG2	2.00	0.44
1:A:671:LEU:HD23	1:A:678:LEU:HD23	2.00	0.44
1:C:580:GLU:O	1:C:581:LYS:CB	2.66	0.43
1:A:495:THR:HA	1:A:521:MET:O	2.19	0.43
1:B:316:LEU:HD11	1:B:362:LYS:HG3	1.99	0.43
1:C:304:ILE:HD12	1:C:308:GLU:CB	2.47	0.43
1:C:523:GLU:O	1:C:526:ASP:HB2	2.17	0.43
1:B:660:LYS:NZ	1:B:660:LYS:CB	2.80	0.43
1:B:486:GLU:C	1:B:488:GLN:H	2.26	0.43
1:C:454:GLN:H	1:C:454:GLN:HG3	1.64	0.43
1:A:318:ASN:HD22	1:A:318:ASN:HA	1.61	0.43
1:A:320:TRP:CD1	1:A:320:TRP:C	2.95	0.43
1:C:549:LEU:HD13	1:C:591:ARG:HH12	1.84	0.43
1:A:327:LYS:HD3	1:A:423:LEU:HB2	2.00	0.43
1:B:495:THR:HG22	1:B:521:MET:HB2	2.01	0.43
1:C:602:SER:CB	1:C:631:LYS:HD2	2.49	0.43
1:A:449:ILE:HD13	1:A:463:LEU:HD11	2.00	0.43
1:B:340:LEU:O	1:B:387:GLY:HA3	2.19	0.43
1:A:694:LEU:O	1:A:696:LEU:N	2.48	0.42
1:B:546:LYS:HA	1:B:601:THR:O	2.19	0.42
1:B:513:LYS:HD2	1:B:593:VAL:HG11	2.01	0.42
1:C:655:ASN:HB3	1:C:656:ASP:H	1.61	0.42
1:A:485:LYS:HE2	1:A:515:GLY:O	2.18	0.42
1:B:508:VAL:O	1:B:512:ARG:HG3	2.20	0.42
1:C:593:VAL:CG2	1:C:594:THR:N	2.83	0.42
1:C:632:LYS:H	1:C:632:LYS:HG2	1.66	0.42
1:A:494:ILE:HB	1:A:544:VAL:CG2	2.49	0.42
1:A:606:TRP:HD1	1:A:610:MET:HG2	1.85	0.42
1:B:578:ILE:C	1:B:580:GLU:N	2.77	0.42
1:C:366:ARG:O	1:C:367:ARG:HB2	2.19	0.41
1:C:671:LEU:HD23	1:C:678:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:LYS:HB2	1:B:633:HIS:CD2	2.54	0.41
1:A:438:TYR:CE2	1:A:442:SER:HB2	2.55	0.41
1:A:478:LYS:O	1:A:482:THR:HG23	2.20	0.41
1:A:547:GLU:HG2	1:A:603:THR:HG23	2.03	0.41
1:A:510:ARG:NH2	1:A:557:GLU:OE2	2.53	0.41
1:A:578:ILE:HG13	1:A:579:LEU:N	2.35	0.41
1:C:366:ARG:C	1:C:367:ARG:HD3	2.45	0.41
1:A:646:LEU:HG	1:A:662:LEU:HD23	2.02	0.41
1:B:349:PHE:O	1:B:349:PHE:CG	2.74	0.41
1:A:610:MET:HA	1:A:610:MET:HE3	2.03	0.41
1:C:498:THR:HG22	1:C:500:ASP:N	2.35	0.41
1:C:509:GLU:HB3	1:C:593:VAL:HG22	2.02	0.41
1:A:574:ILE:O	1:A:578:ILE:HG23	2.21	0.41
1:B:575:MET:HE3	1:B:663:VAL:HG13	2.03	0.40
1:B:589:SER:HB2	1:B:635:GLU:HB3	2.02	0.40
1:A:692:ILE:HD12	1:B:662:LEU:CD1	2.49	0.40
1:B:555:GLU:H	1:B:555:GLU:HG2	1.61	0.40
1:C:597:CYS:HB2	1:C:634:LEU:HD11	2.03	0.40
1:A:394:LEU:HA	1:A:395:PRO:HD3	1.88	0.40
1:A:468:SER:HB2	1:A:512:ARG:HD3	2.04	0.40
1:B:304:ILE:HD12	1:B:308:GLU:HB3	2.02	0.40
1:B:304:ILE:CD1	1:B:308:GLU:HB3	2.52	0.40
1:C:465:TYR:CZ	1:C:521:MET:HE2	2.57	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	364/448 (81%)	344 (94%)	15 (4%)	5 (1%)	9	36
1	B	366/448 (82%)	335 (92%)	26 (7%)	5 (1%)	9	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	361/448 (81%)	323 (90%)	27 (8%)	11 (3%)	3	19
All	All	1091/1344 (81%)	1002 (92%)	68 (6%)	21 (2%)	6	30

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	580	GLU
1	B	376	GLU
1	C	432	GLU
1	A	429	GLU
1	A	696	LEU
1	B	393	ASP
1	C	334	GLN
1	C	374	CYS
1	C	433	ASN
1	A	430	ASP
1	B	406	SER
1	C	581	LYS
1	C	647	ARG
1	C	653	ASP
1	B	374	CYS
1	C	656	ASP
1	C	348	PRO
1	C	585	LYS
1	A	555	GLU
1	B	407	LYS
1	C	548	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	346/412 (84%)	296 (86%)	50 (14%)	3	15
1	B	348/412 (84%)	300 (86%)	48 (14%)	3	17
1	C	343/412 (83%)	296 (86%)	47 (14%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1037/1236 (84%)	892 (86%)	145 (14%)	3 16

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	THR
1	A	300	ASN
1	A	307	GLU
1	A	338	ARG
1	A	340	LEU
1	A	360	ASN
1	A	366	ARG
1	A	367	ARG
1	A	372	ASP
1	A	378	ILE
1	A	383	ASN
1	A	388	VAL
1	A	394	LEU
1	A	413	ARG
1	A	414	LYS
1	A	442	SER
1	A	443	LYS
1	A	447	LEU
1	A	478	LYS
1	A	479	ASP
1	A	486	GLU
1	A	489	LYS
1	A	498	THR
1	A	512	ARG
1	A	525	ILE
1	A	535	GLU
1	A	537	GLU
1	A	559	LYS
1	A	560	LYS
1	A	574	ILE
1	A	578	ILE
1	A	583	VAL
1	A	586	VAL
1	A	593	VAL
1	A	599	ILE
1	A	603	THR
1	A	604	TYR

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Mol	Chain	Res	Type
1	A	606	TRP
1	A	610	MET
1	A	612	ARG
1	A	614	MET
1	A	646	LEU
1	A	657	LYS
1	A	658	SER
1	A	665	LEU
1	A	677	SER
1	A	682	GLN
1	A	692	ILE
1	A	694	LEU
1	A	696	LEU
1	B	296	ILE
1	B	304	ILE
1	B	340	LEU
1	B	346	ARG
1	B	367	ARG
1	B	368	VAL
1	B	376	GLU
1	B	377	LEU
1	B	378	ILE
1	B	388	VAL
1	B	407	LYS
1	B	408	ILE
1	B	411	VAL
1	B	433	ASN
1	B	435	LYS
1	B	443	LYS
1	B	457	LYS
1	B	482	THR
1	B	486	GLU
1	B	501	GLN
1	B	523	GLU
1	B	525	ILE
1	B	535	GLU
1	B	542	VAL
1	B	551	LEU
1	B	555	GLU
1	B	557	GLU
1	B	574	ILE
1	B	577	ASP

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Mol	Chain	Res	Type
1	B	578	ILE
1	B	581	LYS
1	B	595	SER
1	B	603	THR
1	B	604	TYR
1	B	607	THR
1	B	613	ILE
1	B	645	THR
1	B	646	LEU
1	B	647	ARG
1	B	655	ASN
1	B	657	LYS
1	B	661	ASP
1	B	665	LEU
1	B	668	GLU
1	B	678	LEU
1	B	679	GLU
1	B	682	GLN
1	B	692	ILE
1	C	304	ILE
1	C	334	GLN
1	C	340	LEU
1	C	360	ASN
1	C	368	VAL
1	C	372	ASP
1	C	378	ILE
1	C	380	GLU
1	C	394	LEU
1	C	407	LYS
1	C	410	LYS
1	C	418	LYS
1	C	453	SER
1	C	454	GLN
1	C	464	ARG
1	C	478	LYS
1	C	482	THR
1	C	486	GLU
1	C	495	THR
1	C	508	VAL
1	C	525	ILE
1	C	534	LYS
1	C	535	GLU

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Mol	Chain	Res	Type
1	C	547	GLU
1	C	555	GLU
1	C	557	GLU
1	C	566	THR
1	C	574	ILE
1	C	576	LYS
1	C	583	VAL
1	C	584	GLU
1	C	585	LYS
1	C	586	VAL
1	C	588	VAL
1	C	599	ILE
1	C	603	THR
1	C	604	TYR
1	C	614	MET
1	C	632	LYS
1	C	648	GLN
1	C	656	ASP
1	C	657	LYS
1	C	660	LYS
1	C	662	LEU
1	C	678	LEU
1	C	694	LEU
1	C	696	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	A	318	ASN
1	A	334	GLN
1	A	433	ASN
1	A	450	HIS
1	A	570	ASN
1	A	682	GLN
1	B	359	ASN
1	B	450	HIS
1	B	454	GLN
1	B	487	ASN
1	B	501	GLN
1	B	514	HIS
1	B	633	HIS

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Mol	Chain	Res	Type
1	B	655	ASN
1	B	682	GLN
1	C	334	GLN
1	C	433	ASN
1	C	444	ASN
1	C	450	HIS
1	C	487	ASN
1	C	609	ASN
1	C	633	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](#)

3 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	SO4	C	3	-	4,4,4	0.22	0	6,6,6	0.16	0
2	SO4	A	1	-	4,4,4	0.25	0	6,6,6	0.27	0
2	SO4	B	2	-	4,4,4	0.22	0	6,6,6	0.45	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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 [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	372/448 (83%)	-0.35	1 (0%) 90 79	67, 94, 136, 185	0
1	B	374/448 (83%)	-0.28	3 (0%) 82 64	61, 89, 143, 174	0
1	C	369/448 (82%)	-0.03	11 (2%) 52 30	69, 114, 187, 222	0
All	All	1115/1344 (82%)	-0.22	15 (1%) 75 53	61, 98, 161, 222	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	697	GLY	3.5
1	C	630	ALA	3.3
1	C	315	SER	3.2
1	B	613	ILE	3.1
1	A	395	PRO	2.7
1	C	294	LYS	2.4
1	B	294	LYS	2.4
1	C	604	TYR	2.3
1	C	349	PHE	2.2
1	C	611	GLU	2.2
1	C	578	ILE	2.1
1	C	565	LYS	2.1
1	C	587	VAL	2.0
1	C	528	TYR	2.0
1	B	639	ASP	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	SO4	C	3	5/5	0.85	0.08	164,165,165,165	0
2	SO4	A	1	5/5	0.91	0.10	127,128,128,129	0
2	SO4	B	2	5/5	0.92	0.12	120,121,122,123	0

6.5 Other polymers [i](#)

There are no such residues in this entry.