



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:51 AM GMT

PDB ID : 3Q6M
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

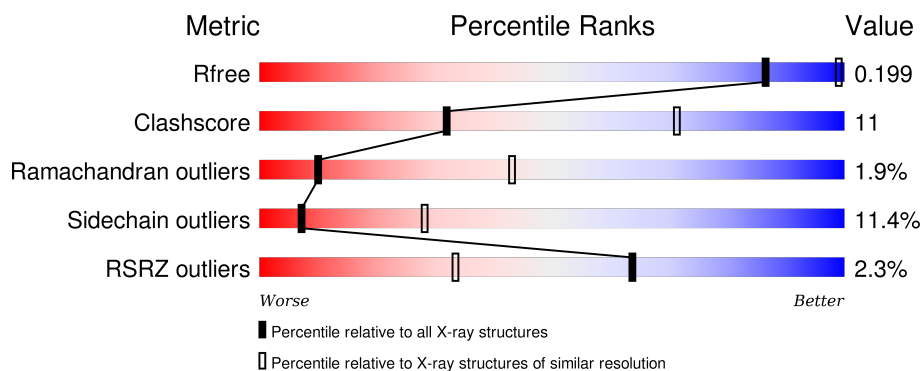
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	448	<div> <div>2%</div> <div>59% 19% 5% 17%</div> </div>
1	B	448	<div> <div>%</div> <div>63% 16% 5% 17%</div> </div>
1	C	448	<div> <div>3%</div> <div>59% 19% • 18%</div> </div>

2 Entry composition

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:

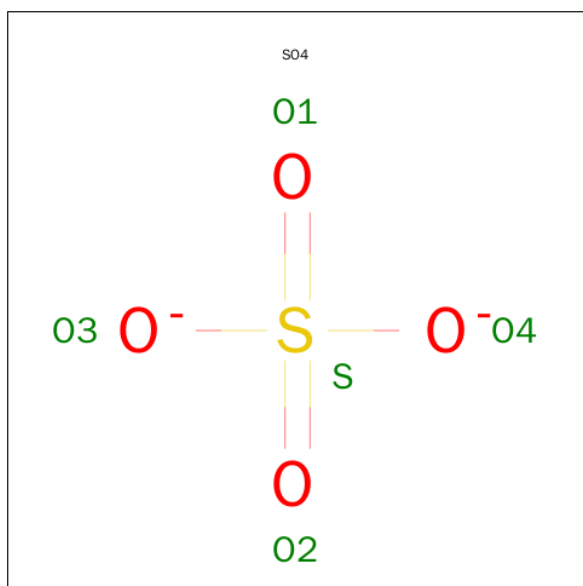
Chain	Residue	Modelled	Actual	Comment	Reference
A	291	ALA	-	EXPRESSION TAG	UNP P07900
A	292	ALA	-	EXPRESSION TAG	UNP P07900
A	733	HIS	-	EXPRESSION TAG	UNP P07900
A	734	HIS	-	EXPRESSION TAG	UNP P07900
A	735	HIS	-	EXPRESSION TAG	UNP P07900
A	736	HIS	-	EXPRESSION TAG	UNP P07900
A	737	HIS	-	EXPRESSION TAG	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	738	HIS	-	EXPRESSION TAG	UNP P07900

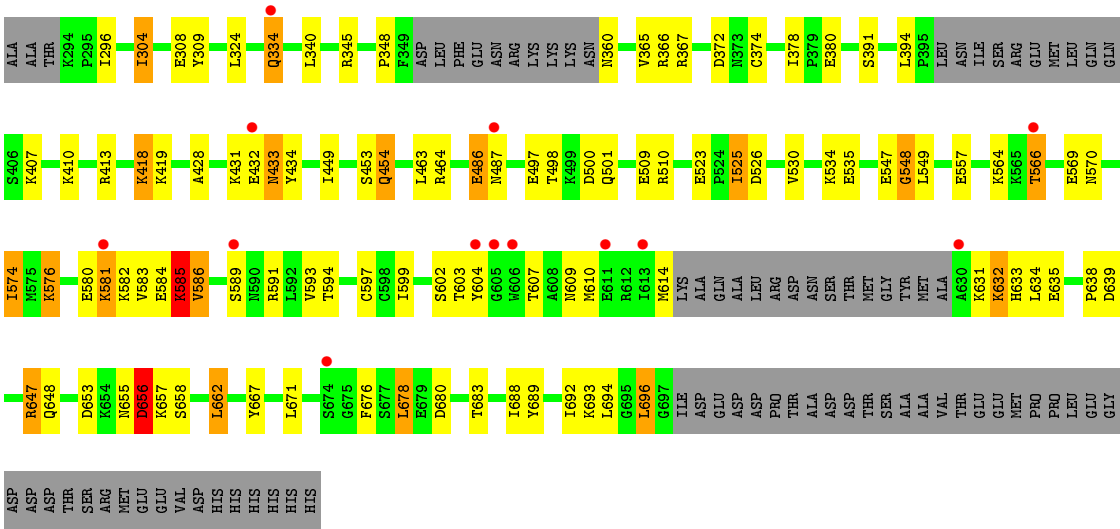
- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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		



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 29.84 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-3.00) 95.0 (29.84-3.00)	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	REFMAC 5.5.0109	Depositor
R, R_{free}	0.209 , 0.252 0.204 , 0.199	Depositor DCC
R_{free} test set	2184 reflections (5.51%)	DCC
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 , 76.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 43622 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.62	0/3120	0.69	0/4188
1	B	0.66	0/3136	0.71	1/4210 (0.0%)
1	C	0.57	0/3094	0.65	1/4154 (0.0%)
All	All	0.61	0/9350	0.68	2/12552 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	646	LEU	CA-CB-CG	7.56	132.69	115.30
1	C	696	LEU	CA-CB-CG	5.52	128.00	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3069	0	3108	72	0
1	B	3085	0	3123	70	0
1	C	3043	0	3081	64	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	197	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 (197) 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:HG3	1:B:367:ARG:HH11	1.15	1.03
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:H	1:C:525:ILE:HD12	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:HD12	1:B:525:ILE:H	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:HG2	1:C:647:ARG:HH11	1.47	0.79
1:B:509:GLU:HB3	1:B:593:VAL:HG22	1.65	0.78
1:A:486:GLU:HA	1:A:486:GLU:OE2	1.85	0.77
1:A:509:GLU:HB3	1:A:593:VAL:HG13	1.67	0.76
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: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:HH11	1:B:346:ARG:HG3	1.52	0.74
1:C:607:THR:H	1:C:610:MET:HE3	1.55	0.72
1:B:655:ASN:ND2	1:B:655:ASN:H	1.87	0.71
1:A:429:GLU:O	1:A:430:ASP:C	2.28	0.71
1:C:688:ILE:O	1:C:692:ILE:HG22	1.91	0.71
1:B:641:SER:O	1:B:645:THR:HG23	1.90	0.71
1:C:304:ILE:HD12	1:C:308:GLU:HB2	1.73	0.71
1:C:525:ILE:H	1:C:525:ILE:CD1	2.03	0.70
1:A:688:ILE:O	1:A:692:ILE:HG23	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:LYS:NZ	1:B:660:LYS:HB3	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:N	1:B:655:ASN:HD22	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:HG3	1:A:614:MET:O	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:296:ILE:HD11	1:C:304:ILE:HD13	1.78	0.66
1:C:607:THR:N	1:C:610:MET:HE3	2.12	0.65
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:431:LYS:C	1:C:433:ASN:H	2.02	0.62
1:A:691:MET:SD	1:B:691:MET:CE	2.88	0.62
1:A:691:MET:SD	1:B:691:MET:HE1	2.40	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:B:509:GLU:OE2	1:B:595:SER:HB2	2.00	0.60
1:A:692:ILE:HD12	1:B:662:LEU:HD11	1.82	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:C:647:ARG:HH12	1:C:648:GLN:HG3	1.67	0.59
1:B:405:GLN:HG3	1:B:406:SER:N	2.16	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
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: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:HB2	1:A:338:ARG:HH11	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:GLY:O	1:A:696:LEU:HD12	2.07	0.55
1:A:447:LEU:O	1:A:451:GLU:HG2	2.06	0.55
1:A:692:ILE:HD11	1:B:666:LEU:HD21	1.88	0.55
1:A:435:LYS:NZ	3:A:100:HOH:O	2.39	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:C:582:LYS:HB3	1:C:667:TYR:CE2	2.43	0.54
1:A:566:THR:HA	1:A:569:GLU:HB2	1.89	0.54
1:C:526:ASP:O	1:C:530:VAL:HG22	2.08	0.54
1:C:689:TYR:HA	1:C:692:ILE:HG22	1.89	0.54
1:C:486:GLU:HA	1:C:486:GLU:OE1	2.06	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:B:304:ILE:HD12	1:B:308:GLU:CB	2.39	0.52
1:A:578:ILE:HD11	1:A:664:ILE:HG13	1.91	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:A:679:GLU:H	1:A:679:GLU:CD	2.14	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:HZ3	1:B:660:LYS:HB3	1.76	0.51
1:C:689:TYR:O	1:C:693:LYS:HB2	2.11	0.51
1:B:610:MET:O	1:B:614:MET:HG2	2.10	0.50
1:B:450:HIS:HD2	1:B:528:TYR:O	1.94	0.50
1:A:691:MET:O	1:A:694:LEU:HB3	2.11	0.50
1:A:684:HIS:CE1	1:A:688:ILE:HD11	2.47	0.50
1:A:602:SER:HB3	1:A:631:LYS:HB2	1.93	0.50
1:C:296:ILE:HD11	1:C:304:ILE:CD1	2.42	0.50
1:B:346:ARG:HG3	1:B:346:ARG:NH1	2.22	0.50
1:C:410:LYS:HZ2	1:C:413:ARG:HD3	1.76	0.50
1:A:580:GLU:HG3	1:A:581:LYS:H	1.77	0.50
1:B:525:ILE:CD1	1:B:525:ILE:H	2.11	0.49
1:A:578:ILE:HD13	1:A:660:LYS:HG3	1.94	0.49
1:A:585:LYS:HG2	1:A:587:VAL:HG13	1.94	0.49
1:A:307:GLU:CD	1:A:307:GLU:H	2.16	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:VAL:HG23	1:C:594:THR:N	2.27	0.49
1:B:604:TYR:HD2	1:B:604:TYR:H	1.58	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: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:HZ2	1:B:660:LYS:HB3	1.80	0.46
1:B:490:HIS:HB3	1:B:542:VAL:CG1	2.45	0.46
1:B:495:THR:HA	1:B:521:MET:O	2.15	0.46
1:A:554:ASP:OD2	1:A:556:GLU:HB3	2.15	0.46
1:C:602:SER:HB2	1:C:633:HIS:HE1	1.80	0.46
1:C:607:THR:HG23	1:C:609:ASN:H	1.81	0.46
1:A:642:ILE:O	1:A:646:LEU:HB2	2.15	0.46
1:A:582:LYS:HD2	1:A:667:TYR:CE2	2.50	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
1:C:431:LYS:C	1:C:433:ASN:N	2.70	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:579:LEU:HD11	1:A:667:TYR:HB2	1.98	0.45
1:A:535:GLU:HB3	1:A:540:THR:HA	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:A:525:ILE:CD1	1:A:525:ILE:H	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:B:578:ILE:C	1:B:580:GLU:H	2.21	0.43
1:C:580:GLU:O	1:C:581:LYS:CB	2.66	0.43
1:A:610:MET:HA	1:A:610:MET:HE3	2.00	0.43
1:A:495:THR:HA	1:A:521:MET:O	2.19	0.43
1:C:304:ILE:HD12	1:C:308:GLU:CB	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:523:GLU:O	1:C:526:ASP:HB2	2.17	0.43
1:B:316:LEU:HD11	1:B:362:LYS:HG3	1.99	0.43
1:B:660:LYS:CB	1:B:660:LYS:NZ	2.80	0.43
1:C:366:ARG:O	1:C:367:ARG:HB2	2.19	0.43
1:C:454:GLN:H	1:C:454:GLN:HG3	1.64	0.43
1:C:549:LEU:HD13	1:C:591:ARG:HH12	1.84	0.43
1:A:318:ASN:HA	1:A:318:ASN:HD22	1.61	0.43
1:C:602:SER:CB	1:C:631:LYS:HD2	2.49	0.43
1:B:495:THR:HG22	1:B:521:MET:HB2	2.01	0.43
1:A:327:LYS:HD3	1:A:423:LEU:HB2	2.00	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:A:579:LEU:O	1:A:580:GLU:C	2.58	0.42
1:C:655:ASN:HB3	1:C:656:ASP:H	1.61	0.42
1:C:593:VAL:CG2	1:C:594:THR:N	2.83	0.42
1:C:632:LYS:HG2	1:C:632:LYS:H	1.66	0.42
1:B:508:VAL:O	1:B:512:ARG:HG3	2.20	0.42
1:A:485:LYS:HE2	1:A:515:GLY:O	2.18	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:C:671:LEU:HD23	1:C:678:LEU:HD23	2.02	0.41
1:B:585:LYS:HB2	1:B:633:HIS:CD2	2.54	0.41
1:B:414:LYS:HZ3	1:B:454:GLN:HE22	1.65	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:578:ILE:HG13	1:A:579:LEU:N	2.35	0.41
1:A:510:ARG:NH2	1:A:557:GLU:OE2	2.53	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:C:509:GLU:HB3	1:C:593:VAL:HG22	2.02	0.41
1:C:498:THR:HG22	1:C:500:ASP:N	2.35	0.41
1:A:574:ILE:O	1:A:578:ILE:HG23	2.21	0.41
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:HG2	1:B:555:GLU:H	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ILE:CD1	1:B:308:GLU:HB3	2.52	0.40
1:B:304:ILE:HD12	1:B:308:GLU:HB3	2.02	0.40
1:A:468:SER:HB2	1:A:512:ARG:HD3	2.04	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%)	14	51
1	B	366/448 (82%)	335 (92%)	26 (7%)	5 (1%)	14	51
1	C	361/448 (81%)	323 (90%)	27 (8%)	11 (3%)	5	29
All	All	1091/1344 (81%)	1002 (92%)	68 (6%)	21 (2%)	10	43

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	305 (88%)	41 (12%)	6	26
1	B	348/412 (84%)	309 (89%)	39 (11%)	7	29
1	C	343/412 (83%)	305 (89%)	38 (11%)	8	29
All	All	1037/1236 (84%)	919 (89%)	118 (11%)	7	28

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	394	LEU
1	A	413	ARG
1	A	414	LYS
1	A	431	LYS
1	A	442	SER
1	A	443	LYS
1	A	447	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	478	LYS
1	A	479	ASP
1	A	486	GLU
1	A	498	THR
1	A	512	ARG
1	A	525	ILE
1	A	535	GLU
1	A	559	LYS
1	A	574	ILE
1	A	578	ILE
1	A	583	VAL
1	A	586	VAL
1	A	593	VAL
1	A	604	TYR
1	A	606	TRP
1	A	610	MET
1	A	612	ARG
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	304	ILE
1	B	340	LEU
1	B	346	ARG
1	B	367	ARG
1	B	374	CYS
1	B	376	GLU
1	B	377	LEU
1	B	378	ILE
1	B	388	VAL
1	B	407	LYS
1	B	411	VAL
1	B	433	ASN
1	B	435	LYS
1	B	443	LYS
1	B	482	THR
1	B	486	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	501	GLN
1	B	525	ILE
1	B	535	GLU
1	B	542	VAL
1	B	551	LEU
1	B	555	GLU
1	B	574	ILE
1	B	576	LYS
1	B	577	ASP
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	645	THR
1	B	646	LEU
1	B	647	ARG
1	B	655	ASN
1	B	661	ASP
1	B	665	LEU
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	372	ASP
1	C	378	ILE
1	C	380	GLU
1	C	394	LEU
1	C	407	LYS
1	C	418	LYS
1	C	453	SER
1	C	454	GLN
1	C	464	ARG
1	C	486	GLU
1	C	487	ASN
1	C	510	ARG
1	C	525	ILE
1	C	534	LYS
1	C	535	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	557	GLU
1	C	566	THR
1	C	574	ILE
1	C	576	LYS
1	C	584	GLU
1	C	585	LYS
1	C	586	VAL
1	C	599	ILE
1	C	603	THR
1	C	604	TYR
1	C	614	MET
1	C	632	LYS
1	C	639	ASP
1	C	656	ASP
1	C	657	LYS
1	C	662	LEU
1	C	678	LEU
1	C	694	LEU
1	C	696	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	A	318	ASN
1	A	334	GLN
1	A	450	HIS
1	A	570	ASN
1	A	682	GLN
1	B	433	ASN
1	B	450	HIS
1	B	454	GLN
1	B	487	ASN
1	B	501	GLN
1	B	514	HIS
1	B	655	ASN
1	B	682	GLN
1	C	360	ASN
1	C	450	HIS
1	C	487	ASN
1	C	504	ASN
1	C	609	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 carbohydrates 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	A	1	-	4,4,4	0.15	0	6,6,6	0.20	0
2	SO4	B	2	-	4,4,4	0.23	0	6,6,6	0.39	0
2	SO4	C	3	-	4,4,4	0.19	0	6,6,6	0.22	0

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	SO4	A	1	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	C	3	-	-	0/0/0/0	0/0/0/0

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 [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	372/448 (83%)	-0.13	8 (2%) 65 35	67, 94, 136, 185	0
1	B	374/448 (83%)	-0.18	5 (1%) 79 53	61, 89, 143, 174	0
1	C	369/448 (82%)	-0.01	13 (3%) 48 21	69, 114, 187, 222	0
All	All	1115/1344 (82%)	-0.10	26 (2%) 64 33	61, 98, 161, 222	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	606	TRP	4.4
1	C	630	ALA	4.4
1	A	395	PRO	4.3
1	C	604	TYR	4.0
1	A	559	LYS	3.7
1	B	630	ALA	3.5
1	A	303	ASP	3.3
1	C	589	SER	3.1
1	B	395	PRO	3.0
1	B	373	ASN	2.9
1	C	581	LYS	2.5
1	A	604	TYR	2.5
1	A	606	TRP	2.5
1	C	432	GLU	2.4
1	C	674	SER	2.4
1	B	614	MET	2.3
1	A	334	GLN	2.3
1	C	334	GLN	2.3
1	C	566	THR	2.3
1	A	630	ALA	2.2
1	C	613	ILE	2.2
1	B	375	GLU	2.2
1	A	614	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	487	ASN	2.1
1	C	605	GLY	2.1
1	C	611	GLU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	1	5/5	0.92	0.14	-	127,128,128,129	0
2	SO4	B	2	5/5	0.90	0.19	-	120,121,122,123	0
2	SO4	C	3	5/5	0.70	0.32	-	164,165,165,165	0

6.5 Other polymers [i](#)

There are no such residues in this entry.