Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 06:02 PM EDT

PDB ID	:	1DD1
Title	:	CRYSTAL STRUCTURE ANALYSIS OF THE SMAD4 ACTIVE FRAGMENT
Authors	:	Qin, B.Y.; Lam, S.W.; Lin, K.
Deposited on	:	1999-11-05
Resolution	:	2.62 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:

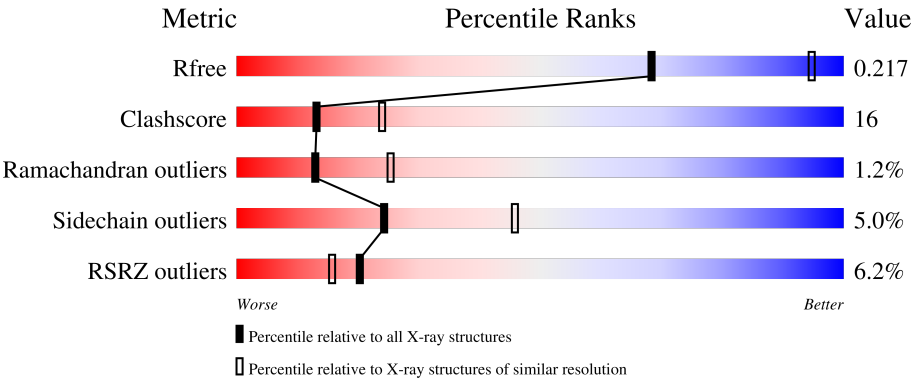
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 <=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	268	4% 63% 17% • 18%
1	B	268	6% 66% 24% • 7%
1	C	268	6% 63% 25% • 10%

2 Entry composition

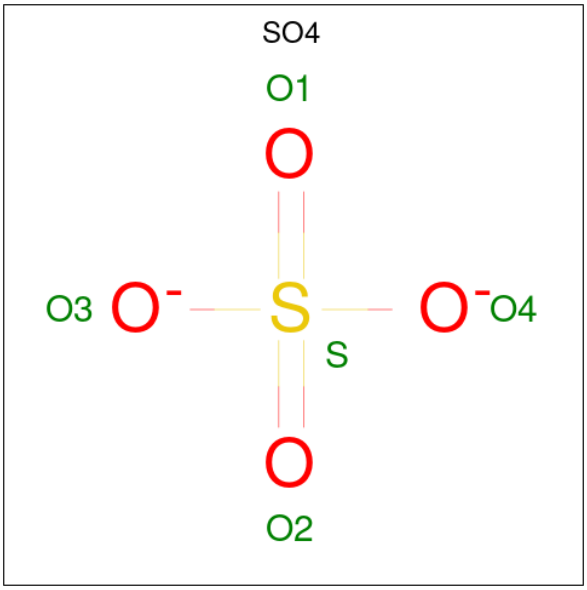
There are 3 unique types of molecules in this entry. The entry contains 5889 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SMAD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1738	1099	315	311	13			
1	B	249	Total	C	N	O	S	0	1	0
			1938	1224	347	354	13			
1	C	241	Total	C	N	O	S	0	0	0
			1866	1176	337	340	13			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 3 is water.

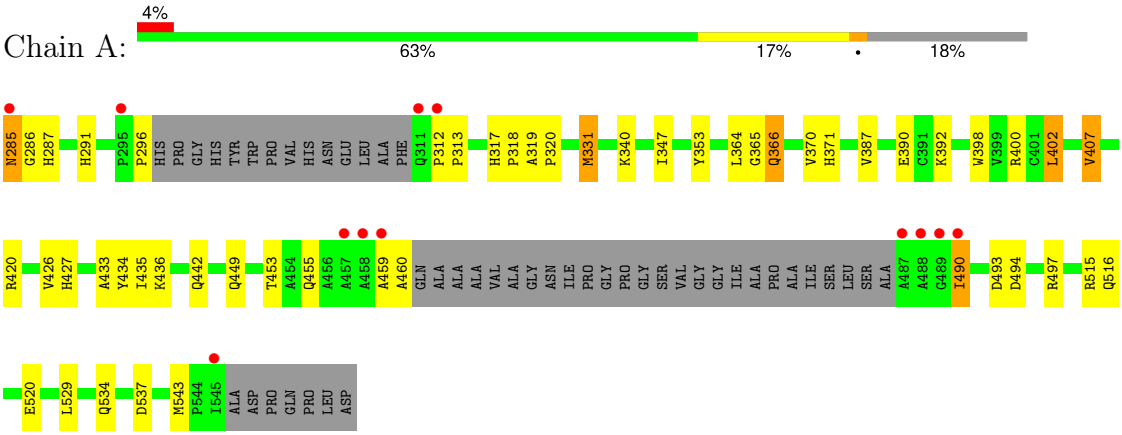
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	106	Total O 106 106	0	0
3	B	111	Total O 111 111	0	0
3	C	85	Total O 85 85	0	0

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.

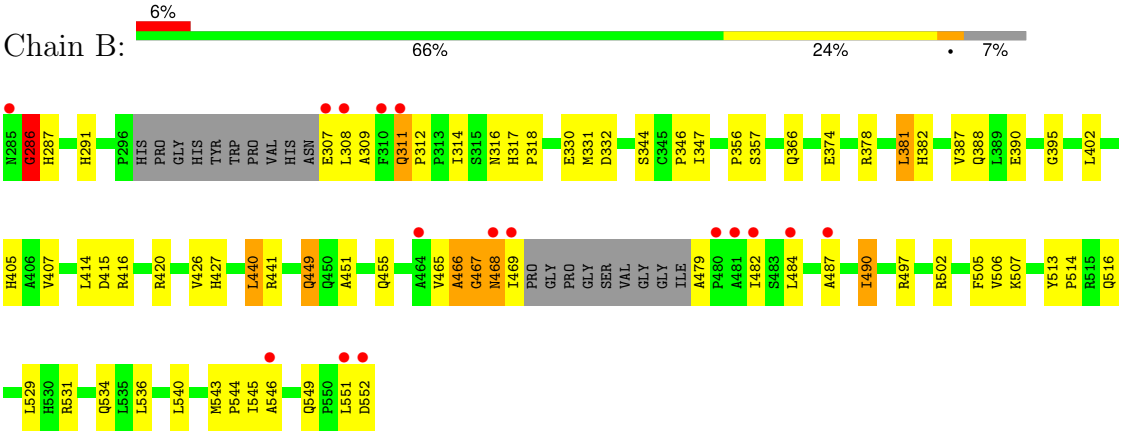
• Molecule 1: SMAD4

Chain A:



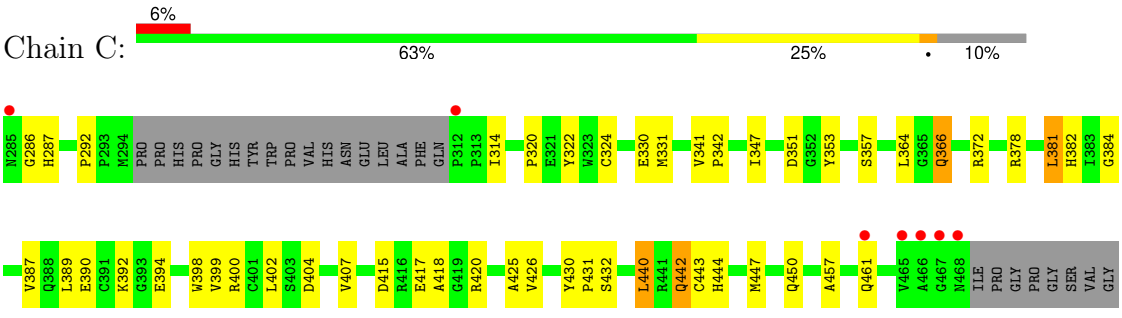
• Molecule 1: SMAD4

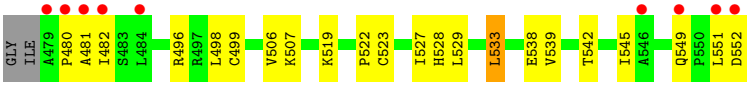
Chain B:



• Molecule 1: SMAD4

Chain C:




GLY
ILE
A479
P480
A481
I482
S483
L484
R496
R497
L498
C499
V506
K507
K519
P522
C523
I527
H528
L529
L533
E538
V539
T542
I545
A546
Q549
P550
L551
D552

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	142.43Å 142.43Å 195.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.62 70.14 – 2.62	Depositor EDS
% Data completeness (in resolution range)	92.9 (100.00-2.62) 92.9 (70.14-2.62)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.62Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.175 0.173 , 0.217	Depositor DCC
R_{free} test set	1468 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	37.0	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 71.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.018 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5889	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.36	0/1786	0.61	0/2427
1	B	0.41	0/1990	0.69	2/2708 (0.1%)
1	C	0.37	0/1915	0.61	0/2603
All	All	0.38	0/5691	0.64	2/7738 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	286	GLY	N-CA-C	7.39	131.58	113.10
1	B	467	GLY	N-CA-C	5.11	125.86	113.10

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	1738	0	1689	50	0
1	B	1938	0	1880	77	0
1	C	1866	0	1814	56	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
2	C	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	106	0	0	9	0
3	B	111	0	0	7	0
3	C	85	0	0	9	0
All	All	5889	0	5383	179	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 16.

All (179) 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:287:HIS:HA	1:B:420:ARG:NH2	1.70	1.07
1:B:287:HIS:HA	1:B:420:ARG:HH21	1.14	1.05
1:B:465:VAL:C	1:B:467:GLY:H	1.55	1.00
1:C:417:GLU:HB2	3:C:640:HOH:O	1.61	1.00
1:A:287:HIS:HA	1:A:420:ARG:HH21	1.26	0.97
1:B:287:HIS:CA	1:B:420:ARG:HH21	1.86	0.89
1:B:490:ILE:HG23	3:B:631:HOH:O	1.76	0.86
1:B:465:VAL:C	1:B:467:GLY:N	2.29	0.84
1:B:484:LEU:HB2	1:B:551:LEU:HD21	1.61	0.83
1:C:420:ARG:HH11	1:C:420:ARG:HB3	1.43	0.82
1:B:314:ILE:HD12	1:B:440:LEU:HD13	1.61	0.82
1:A:449:GLN:O	1:A:453:THR:HG23	1.81	0.79
1:B:490:ILE:HG12	3:B:663:HOH:O	1.82	0.79
1:A:366:GLN:H	1:A:366:GLN:HE21	1.31	0.79
1:A:490:ILE:HG23	1:A:494:ASP:HB2	1.66	0.78
1:B:308:LEU:HD11	1:B:311:GLN:OE1	1.84	0.78
1:A:366:GLN:H	1:A:366:GLN:NE2	1.85	0.75
1:C:506:VAL:HB	3:C:629:HOH:O	1.86	0.75
1:B:551:LEU:N	1:B:551:LEU:HD22	2.01	0.74
1:B:455:GLN:HE21	1:B:544:PRO:HD2	1.52	0.74
1:B:466:ALA:HB2	1:B:551:LEU:HD12	1.71	0.73
1:B:287:HIS:CA	1:B:420:ARG:NH2	2.49	0.72
1:A:392:LYS:HD2	1:A:398:TRP:NE1	2.05	0.71
1:B:307:GLU:O	1:B:307:GLU:HG3	1.90	0.71
1:C:420:ARG:HB3	1:C:420:ARG:NH1	2.05	0.71
1:C:507:LYS:HG2	3:C:629:HOH:O	1.92	0.69
1:C:378:ARG:O	1:C:381:LEU:HB2	1.93	0.68
1:A:516:GLN:HB2	3:A:659:HOH:O	1.94	0.68
1:C:545:ILE:HD12	1:C:545:ILE:H	1.59	0.67
1:B:469:ILE:HG23	1:B:479:ALA:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:PRO:O	1:C:432:SER:HB2	1.94	0.65
1:B:465:VAL:O	1:B:467:GLY:N	2.30	0.64
1:A:287:HIS:CA	1:A:420:ARG:HH21	2.04	0.63
1:B:378:ARG:O	1:B:381:LEU:HB2	1.99	0.61
1:C:387:VAL:CG1	1:C:407:VAL:HG21	2.30	0.61
1:C:549:GLN:O	1:C:549:GLN:HG2	2.01	0.60
1:A:493:ASP:HB3	3:A:637:HOH:O	2.01	0.60
1:B:312:PRO:O	1:B:441:ARG:NH2	2.34	0.60
1:C:286:GLY:O	1:C:420:ARG:NE	2.35	0.60
1:B:549:GLN:O	1:B:551:LEU:HD22	2.03	0.59
1:B:502:ARG:NH1	3:B:586:HOH:O	2.32	0.59
1:B:551:LEU:N	1:B:551:LEU:CD2	2.65	0.58
1:A:287:HIS:HA	1:A:420:ARG:NH2	2.09	0.58
1:A:317:HIS:HE1	3:C:592:HOH:O	1.88	0.57
1:C:287:HIS:HE1	1:C:426:VAL:HG23	1.68	0.57
1:A:291:HIS:HE1	1:A:427:HIS:HD2	1.52	0.57
1:C:482:ILE:O	1:C:551:LEU:HG	2.05	0.57
1:A:435:ILE:HD12	1:A:435:ILE:N	2.19	0.56
1:B:287:HIS:HE1	1:B:426:VAL:HG23	1.71	0.56
1:B:415:ASP:OD1	1:B:427:HIS:HE1	1.89	0.56
1:B:307:GLU:C	1:B:309:ALA:H	2.09	0.55
1:B:388:GLN:HG3	1:B:402:LEU:HD11	1.89	0.55
1:A:366:GLN:HE21	1:A:366:GLN:N	2.02	0.55
1:B:286:GLY:O	1:B:420:ARG:NH2	2.39	0.55
1:B:366:GLN:HA	1:C:496:ARG:HD3	1.89	0.54
1:B:374:GLU:O	1:B:378:ARG:HG2	2.07	0.54
1:B:356:PRO:HD3	1:C:533:LEU:HB3	1.90	0.53
1:A:285:ASN:N	1:A:285:ASN:HD22	2.05	0.53
1:C:457:ALA:O	1:C:461:GLN:HG3	2.09	0.53
1:B:449:GLN:NE2	3:B:662:HOH:O	2.42	0.53
1:C:292:PRO:HA	1:C:430:TYR:HB2	1.90	0.53
1:C:287:HIS:CE1	1:C:426:VAL:HG23	2.43	0.53
1:C:499:CYS:CB	1:C:533:LEU:HD13	2.38	0.53
1:A:285:ASN:O	1:A:286:GLY:C	2.47	0.53
1:B:516:GLN:NE2	1:B:516:GLN:HA	2.24	0.53
1:C:372:ARG:HD2	3:C:557:HOH:O	2.08	0.53
1:B:469:ILE:HG23	1:B:479:ALA:CB	2.39	0.52
1:A:285:ASN:N	1:A:285:ASN:ND2	2.57	0.52
1:B:449:GLN:HE21	1:B:449:GLN:HA	1.73	0.52
1:A:537:ASP:OD2	1:C:353:TYR:HB3	2.09	0.52
1:B:414:LEU:HB3	1:B:427:HIS:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASP:OD1	1:C:425:ALA:HB3	2.09	0.52
1:B:484:LEU:CB	1:B:551:LEU:HD21	2.36	0.51
1:B:308:LEU:HD11	1:B:311:GLN:CD	2.31	0.51
1:B:536:LEU:O	1:B:540:LEU:HG	2.11	0.51
1:C:482:ILE:HB	1:C:551:LEU:HD12	1.93	0.51
1:B:451:ALA:O	1:B:543:MET:HE1	2.11	0.51
1:A:392:LYS:HD2	1:A:398:TRP:CD1	2.45	0.51
1:A:434:TYR:C	1:A:435:ILE:HD12	2.31	0.50
1:C:314:ILE:N	1:C:314:ILE:HD12	2.26	0.50
1:A:312:PRO:HB3	1:A:313:PRO:HD2	1.92	0.50
1:A:291:HIS:HE1	1:A:427:HIS:CD2	2.29	0.50
1:B:455:GLN:HB2	1:B:543:MET:HE1	1.93	0.50
1:B:484:LEU:HD12	1:B:551:LEU:HG	1.94	0.50
1:B:311:GLN:HG2	1:B:311:GLN:O	2.09	0.50
1:B:449:GLN:HE21	1:B:449:GLN:CA	2.23	0.50
1:C:392:LYS:HD2	1:C:398:TRP:NE1	2.26	0.50
1:A:347:ILE:HG12	1:A:390:GLU:HG3	1.94	0.49
1:A:370:VAL:HG13	3:A:612:HOH:O	2.11	0.49
1:A:287:HIS:HE1	1:A:426:VAL:HG23	1.76	0.49
1:A:317:HIS:CD2	1:A:318:PRO:HD2	2.47	0.49
1:B:317:HIS:ND1	1:B:318:PRO:HD2	2.27	0.49
1:B:455:GLN:HB2	1:B:543:MET:CE	2.43	0.49
1:B:465:VAL:HG23	1:B:484:LEU:HD11	1.93	0.49
1:B:469:ILE:HG12	1:B:479:ALA:HB2	1.93	0.49
1:C:347:ILE:HG12	1:C:390:GLU:HG3	1.94	0.48
1:C:545:ILE:HD12	1:C:545:ILE:N	2.28	0.48
1:A:387:VAL:HG11	1:A:407:VAL:HG21	1.95	0.48
1:B:287:HIS:CE1	1:B:426:VAL:HG23	2.47	0.48
1:C:499:CYS:HB2	1:C:533:LEU:HD13	1.95	0.48
1:B:311:GLN:HG3	1:B:441:ARG:NH2	2.29	0.48
1:A:296:PRO:HD3	3:A:608:HOH:O	2.14	0.48
1:C:420:ARG:HD3	1:C:425:ALA:HB2	1.95	0.48
1:A:420:ARG:NH1	3:A:594:HOH:O	2.40	0.47
1:C:538:GLU:O	1:C:542:THR:HG23	2.13	0.47
1:B:468:ASN:C	1:B:468:ASN:HD22	2.17	0.47
1:C:382:HIS:HB2	1:C:506:VAL:HG21	1.98	0.46
1:C:390:GLU:OE2	1:C:392:LYS:HE2	2.15	0.46
1:C:366:GLN:HE21	1:C:366:GLN:HB2	1.48	0.46
1:C:400:ARG:HD2	1:C:402:LEU:HD21	1.96	0.46
1:B:497:ARG:HD2	3:B:619:HOH:O	2.14	0.46
1:C:330:GLU:HA	1:C:522:PRO:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ARG:HH11	1:A:497:ARG:HG2	1.80	0.46
1:B:466:ALA:CB	1:B:551:LEU:HD12	2.44	0.46
3:B:641:HOH:O	1:C:519:LYS:HD3	2.16	0.46
1:A:433:ALA:HB1	1:A:435:ILE:CD1	2.45	0.46
1:B:549:GLN:O	1:B:551:LEU:CD2	2.64	0.46
1:B:469:ILE:HA	1:B:479:ALA:HB2	1.98	0.46
1:B:487:ALA:HB3	3:B:631:HOH:O	2.15	0.46
1:B:455:GLN:NE2	1:B:544:PRO:HD2	2.26	0.46
1:C:443:CYS:O	1:C:447:MET:HG3	2.16	0.45
1:B:311:GLN:CG	1:B:441:ARG:NH2	2.79	0.45
1:C:482:ILE:HB	1:C:551:LEU:CD1	2.45	0.45
1:A:317:HIS:CE1	3:C:592:HOH:O	2.65	0.45
1:C:320:PRO:HB2	1:C:322:TYR:O	2.16	0.45
1:C:394:GLU:HB3	1:C:440:LEU:HD12	1.99	0.45
1:B:468:ASN:C	1:B:468:ASN:ND2	2.70	0.45
1:C:351:ASP:HB2	1:C:384:GLY:O	2.17	0.45
1:A:287:HIS:CE1	1:A:426:VAL:HG23	2.52	0.45
1:A:435:ILE:CG2	1:A:436:LYS:N	2.80	0.45
1:A:387:VAL:CG1	1:A:407:VAL:HG21	2.47	0.44
1:A:490:ILE:HG23	1:A:494:ASP:CB	2.44	0.44
1:B:347:ILE:HG12	1:B:390:GLU:HG3	1.98	0.44
1:B:449:GLN:NE2	1:B:449:GLN:HA	2.33	0.44
3:A:660:HOH:O	1:C:357:SER:HB2	2.18	0.44
1:A:435:ILE:HG22	1:A:436:LYS:N	2.32	0.44
1:C:545:ILE:H	1:C:545:ILE:CD1	2.28	0.44
1:A:320:PRO:HG3	1:A:534:GLN:OE1	2.17	0.43
1:B:330:GLU:O	1:B:331:MET:HB2	2.18	0.43
1:A:340:LYS:NZ	3:A:581:HOH:O	2.45	0.43
1:B:344:SER:O	1:B:346:PRO:HD3	2.19	0.43
1:B:308:LEU:CD1	1:B:311:GLN:NE2	2.82	0.43
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.64	0.43
1:B:286:GLY:C	1:B:420:ARG:HH21	2.22	0.43
1:A:353:TYR:O	1:A:365:GLY:HA3	2.19	0.43
1:C:480:PRO:HB3	1:C:552:ASP:HA	1.99	0.42
1:B:382:HIS:HB3	1:B:405:HIS:CD2	2.54	0.42
1:B:543:MET:HA	1:B:544:PRO:HD3	1.90	0.42
1:C:442:GLN:NE2	3:C:575:HOH:O	2.53	0.42
1:B:291:HIS:NE2	1:B:427:HIS:HD2	2.18	0.42
1:A:455:GLN:HE22	1:A:543:MET:HG2	1.84	0.42
1:B:308:LEU:CD1	1:B:311:GLN:CD	2.87	0.42
1:C:324:CYS:HA	1:C:528:HIS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:GLU:O	1:C:331:MET:HB2	2.20	0.42
1:B:513:TYR:HB3	1:B:514:PRO:HD2	2.01	0.42
1:B:531:ARG:HA	1:B:534:GLN:OE1	2.20	0.42
1:A:366:GLN:NE2	1:A:366:GLN:N	2.62	0.42
1:B:387:VAL:HG11	1:B:407:VAL:HG21	2.01	0.41
1:A:371:HIS:HE1	1:B:332:ASP:OD2	2.03	0.41
1:A:400:ARG:HG2	1:A:402:LEU:HD13	2.02	0.41
1:A:515:ARG:NE	3:A:638:HOH:O	2.43	0.41
1:B:387:VAL:CG1	1:B:407:VAL:HG21	2.50	0.41
1:C:418:ALA:HB2	3:C:639:HOH:O	2.21	0.41
1:B:469:ILE:HG12	1:B:479:ALA:CB	2.49	0.41
1:C:389:LEU:CD2	1:C:399:VAL:HG22	2.51	0.41
1:A:400:ARG:HG2	1:A:402:LEU:CD1	2.50	0.41
1:A:520:GLU:CD	3:A:659:HOH:O	2.60	0.41
1:C:447:MET:HE3	1:C:539:VAL:HG21	2.02	0.41
1:A:459:ALA:O	1:A:460:ALA:C	2.59	0.40
1:C:444:HIS:HA	1:C:447:MET:HE2	2.02	0.40
1:A:433:ALA:HB1	1:A:435:ILE:HD11	2.04	0.40
1:C:341:VAL:HA	1:C:342:PRO:HD3	1.89	0.40
1:C:420:ARG:HH11	1:C:420:ARG:CB	2.24	0.40
1:B:552:ASP:CG	1:B:552:ASP:O	2.58	0.40
1:C:404:ASP:HB2	3:C:565:HOH:O	2.22	0.40
1:A:319:ALA:HA	1:A:320:PRO:HD3	1.94	0.40
1:B:505:PHE:O	1:B:507:LYS:N	2.44	0.40
1:C:381:LEU:HA	1:C:381:LEU:HD13	1.84	0.40
1:C:450:GLN:OE1	1:C:498:LEU:HD11	2.21	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	215/268 (80%)	206 (96%)	8 (4%)	1 (0%)	29 50
1	B	244/268 (91%)	223 (91%)	15 (6%)	6 (2%)	5 9
1	C	235/268 (88%)	222 (94%)	12 (5%)	1 (0%)	34 55
All	All	694/804 (86%)	651 (94%)	35 (5%)	8 (1%)	13 25

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	286	GLY
1	B	466	ALA
1	B	546	ALA
1	B	357	SER
1	A	331	MET
1	C	481	ALA
1	B	395	GLY
1	B	506	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	185/217 (85%)	176 (95%)	9 (5%)	25 46
1	B	204/217 (94%)	193 (95%)	11 (5%)	22 42
1	C	196/217 (90%)	187 (95%)	9 (5%)	27 50
All	All	585/651 (90%)	556 (95%)	29 (5%)	24 46

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	ASN
1	A	331	MET
1	A	364	LEU
1	A	366	GLN
1	A	402	LEU

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Mol	Chain	Res	Type
1	A	407	VAL
1	A	442	GLN
1	A	490	ILE
1	A	529	LEU
1	B	311	GLN
1	B	316	ASN
1	B	381	LEU
1	B	416	ARG
1	B	440	LEU
1	B	449	GLN
1	B	468	ASN
1	B	482	ILE
1	B	490	ILE
1	B	529	LEU
1	B	545	ILE
1	C	364	LEU
1	C	366	GLN
1	C	381	LEU
1	C	440	LEU
1	C	442	GLN
1	C	523	CYS
1	C	527	ILE
1	C	529	LEU
1	C	533	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	HIS
1	A	291	HIS
1	A	334	GLN
1	A	366	GLN
1	A	371	HIS
1	A	382	HIS
1	A	388	GLN
1	A	427	HIS
1	A	455	GLN
1	B	287	HIS
1	B	289	GLN
1	B	311	GLN
1	B	316	ASN
1	B	334	GLN

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Mol	Chain	Res	Type
1	B	388	GLN
1	B	405	HIS
1	B	410	GLN
1	B	427	HIS
1	B	442	GLN
1	B	446	GLN
1	B	449	GLN
1	B	450	GLN
1	B	455	GLN
1	B	468	ASN
1	B	516	GLN
1	B	549	GLN
1	C	287	HIS
1	C	334	GLN
1	C	366	GLN
1	C	427	HIS
1	C	442	GLN
1	C	446	GLN
1	C	449	GLN
1	C	455	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

9 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	B	554	-	4,4,4	0.28	0	6,6,6	0.22	0
2	SO4	B	553	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SO4	A	553	-	4,4,4	0.41	0	6,6,6	0.08	0
2	SO4	A	554	-	4,4,4	0.38	0	6,6,6	0.10	0
2	SO4	C	556	-	4,4,4	0.36	0	6,6,6	0.16	0
2	SO4	B	555	-	4,4,4	0.41	0	6,6,6	0.10	0
2	SO4	C	554	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	C	555	-	4,4,4	0.36	0	6,6,6	0.10	0
2	SO4	C	553	-	4,4,4	0.31	0	6,6,6	0.13	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, 95^{th} 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	221/268 (82%)	0.01	12 (5%)	25	20	20, 37, 90, 115	1 (0%)
1	B	249/268 (92%)	0.07	16 (6%)	19	15	17, 40, 105, 133	1 (0%)
1	C	241/268 (89%)	-0.01	16 (6%)	18	14	19, 38, 93, 128	1 (0%)
All	All	711/804 (88%)	0.02	44 (6%)	20	16	17, 38, 98, 133	3 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	487	ALA	8.1
1	A	488	ALA	5.9
1	B	285	ASN	5.7
1	B	469	ILE	5.2
1	B	307	GLU	4.8
1	C	551	LEU	4.5
1	A	285	ASN	4.5
1	B	551	LEU	4.3
1	A	490	ILE	4.2
1	B	552	ASP	4.1
1	C	285	ASN	4.0
1	B	480	PRO	3.9
1	C	552	ASP	3.8
1	C	480	PRO	3.6
1	B	308	LEU	3.4
1	A	311	GLN	3.4
1	C	546	ALA	3.4
1	A	312	PRO	3.3
1	A	489	GLY	3.3
1	B	546	ALA	3.1
1	B	311	GLN	3.1
1	C	468	ASN	3.0
1	B	487	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	468	ASN	2.9
1	C	467	GLY	2.8
1	C	481	ALA	2.6
1	A	457	ALA	2.5
1	B	481	ALA	2.5
1	B	482	ILE	2.4
1	C	465	VAL	2.4
1	C	549	GLN	2.3
1	C	484	LEU	2.2
1	A	295	PRO	2.2
1	B	484	LEU	2.2
1	C	482	ILE	2.2
1	C	312	PRO	2.2
1	B	310	PHE	2.2
1	A	458	ALA	2.2
1	A	459	ALA	2.2
1	A	545	ILE	2.1
1	C	466	ALA	2.1
1	C	461	GLN	2.1
1	B	464	ALA	2.1
1	C	479	ALA	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 monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
2	SO4	B	555	5/5	0.77	0.24	104,104,105,106	5
2	SO4	C	556	5/5	0.86	0.23	100,100,100,101	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	553	5/5	0.89	0.27	114,114,115,115	0
2	SO4	A	554	5/5	0.92	0.26	93,95,95,95	0
2	SO4	C	555	5/5	0.94	0.41	98,98,99,99	5
2	SO4	A	553	5/5	0.96	0.20	96,96,97,97	0
2	SO4	C	554	5/5	0.96	0.17	92,92,93,94	5
2	SO4	B	554	5/5	0.98	0.13	65,68,72,72	0
2	SO4	C	553	5/5	0.99	0.15	38,39,44,46	0

6.5 Other polymers (i)

There are no such residues in this entry.