Full wwPDB X-ray Structure Validation Report (i)

Mar 19, 2024 – 06:13 pm GMT

PDB ID	:	2XHV
Title	:	HCV-J4 NS5B Polymerase Point Mutant Orthorhombic Crystal Form
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Deposited on	:	2010-06-21
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

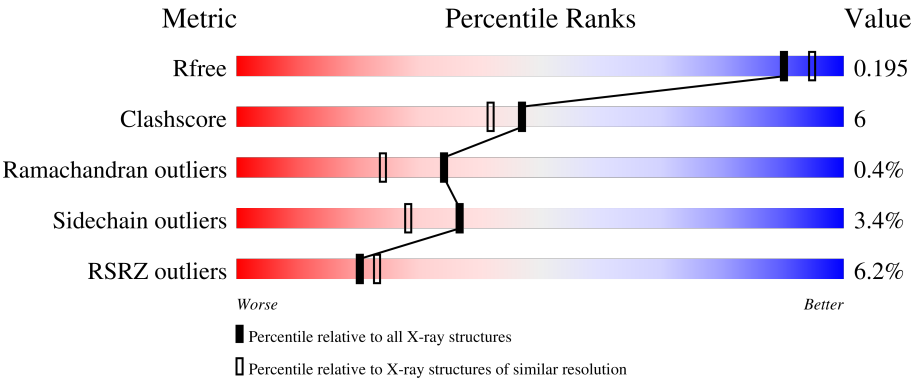
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	579	9% 82% 14%
1	B	579	3% 85% 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9656 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.

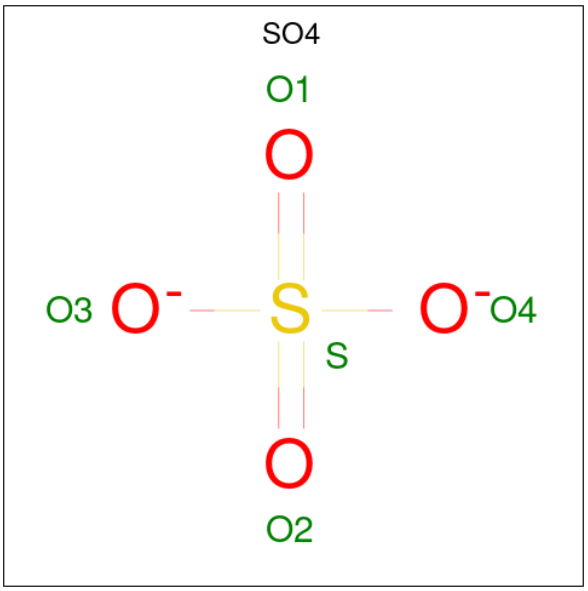
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	3	0
			4402	2772	777	821	32			
1	B	563	Total	C	N	O	S	0	8	0
			4430	2793	783	821	33			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP O92972
A	556	LYS	SER	engineered mutation	UNP O92972
A	571	LEU	-	expression tag	UNP O92972
A	572	GLU	-	expression tag	UNP O92972
A	573	HIS	-	expression tag	UNP O92972
A	574	HIS	-	expression tag	UNP O92972
A	575	HIS	-	expression tag	UNP O92972
A	576	HIS	-	expression tag	UNP O92972
A	577	HIS	-	expression tag	UNP O92972
A	578	HIS	-	expression tag	UNP O92972
B	0	ALA	-	expression tag	UNP O92972
B	556	LYS	SER	engineered mutation	UNP O92972
B	571	LEU	-	expression tag	UNP O92972
B	572	GLU	-	expression tag	UNP O92972
B	573	HIS	-	expression tag	UNP O92972
B	574	HIS	-	expression tag	UNP O92972
B	575	HIS	-	expression tag	UNP O92972
B	576	HIS	-	expression tag	UNP O92972
B	577	HIS	-	expression tag	UNP O92972
B	578	HIS	-	expression tag	UNP O92972

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 10 8 2	0	1
2	A	1	Total O S 20 16 4	0	1
2	A	1	Total O S 10 8 2	0	1
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 10 8 2	0	1
2	B	1	Total O S 20 16 4	0	1
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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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	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is water.

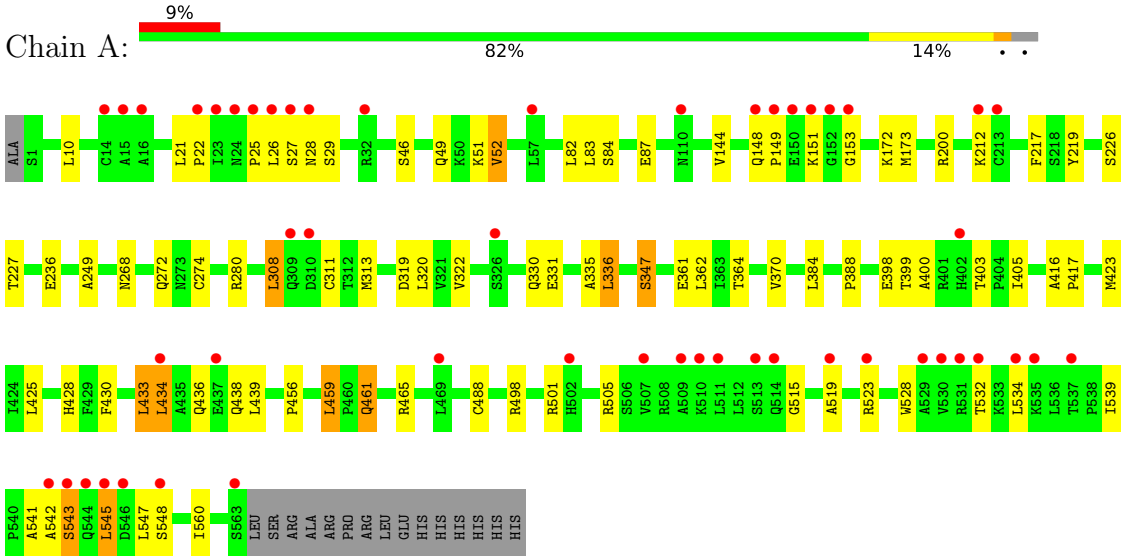
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	278	Total O 278 278	0	0
4	B	409	Total O 409 409	0	0

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.

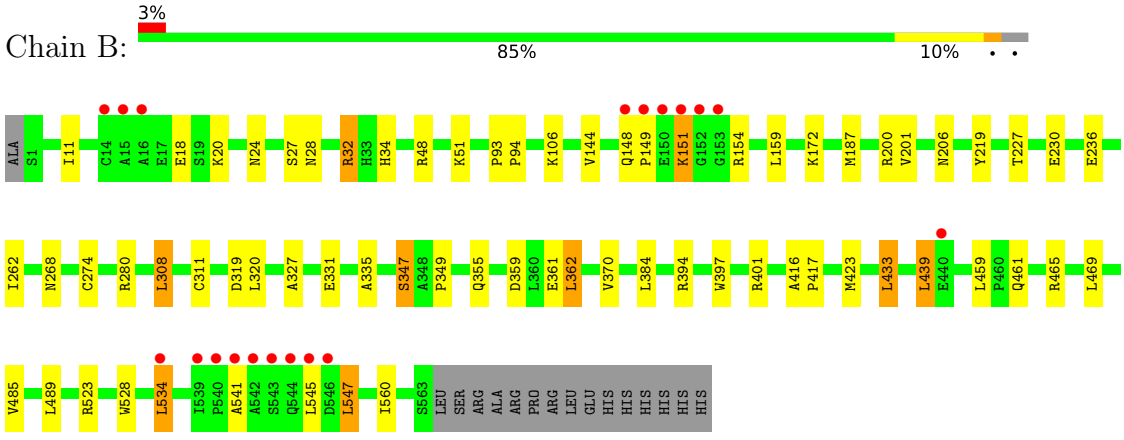
• Molecule 1: RNA-directed RNA polymerase

Chain A:



• Molecule 1: RNA-directed RNA polymerase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.74Å 107.69Å 133.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.67 – 1.90 34.67 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (34.67-1.90) 98.6 (34.67-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 1.89Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.171 , 0.200 0.167 , 0.195	Depositor DCC
R_{free} test set	5945 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9656	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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, MG

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	0.33	0/4504	0.49	0/6111
1	B	0.37	0/4547	0.52	0/6168
All	All	0.35	0/9051	0.51	0/12279

There are no bond length outliers.

There are no bond angle outliers.

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	4402	0	4420	62	0
1	B	4430	0	4471	49	0
2	A	65	0	0	1	0
2	B	70	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	278	0	0	1	0
4	B	409	0	0	4	0
All	All	9656	0	8891	110	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 (110) 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:A:52:VAL:HG22	1:A:226:SER:OG	1.64	0.96
1:B:187:MET:SD	4:B:2177:HOH:O	2.30	0.88
1:A:268:ASN:HD21	1:A:272:GLN:HE21	1.23	0.85
1:B:28:ASN:O	1:B:32[B]:ARG:HD2	1.79	0.83
1:A:398:GLU:HG2	1:A:403:THR:HG21	1.59	0.82
1:B:201:VAL:HG22	1:B:384:LEU:HG	1.62	0.81
1:B:230:GLU:HB3	1:B:262[B]:ILE:HD11	1.67	0.74
1:B:201:VAL:CG2	1:B:384:LEU:HG	2.20	0.71
1:B:308:LEU:HB3	1:B:311:CYS:SG	2.34	0.68
1:B:230:GLU:HG2	1:B:262[B]:ILE:HG12	1.76	0.67
1:A:200:ARG:HD3	1:A:384:LEU:HD11	1.76	0.66
1:B:545:LEU:HG	1:B:547:LEU:HD13	1.77	0.66
1:A:465:ARG:HH11	1:A:545:LEU:HD12	1.60	0.65
1:A:498:ARG:HD3	1:B:206:ASN:HD21	1.63	0.64
1:A:27:SER:HB2	1:A:399:THR:HG21	1.81	0.63
1:A:27:SER:CB	1:A:399:THR:HG21	2.29	0.62
1:B:154:ARG:HD3	4:B:2158:HOH:O	2.00	0.62
1:A:542:ALA:O	1:A:543:SER:HB3	2.00	0.61
1:B:148:GLN:HG3	1:B:149:PRO:HD2	1.82	0.60
1:A:465:ARG:NH1	1:A:545:LEU:HD12	2.16	0.60
1:A:461:GLN:HG2	1:A:541:ALA:HB3	1.82	0.59
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.84	0.58
1:A:236[A]:GLU:OE2	1:A:280:ARG:NH2	2.34	0.57
1:A:25:PRO:HG2	1:A:28:ASN:HB2	1.86	0.57
1:A:361:GLU:HG3	1:A:370:VAL:O	2.04	0.57
1:A:308:LEU:HB3	1:A:311:CYS:SG	2.45	0.56
1:A:542:ALA:O	1:A:543:SER:CB	2.53	0.56
1:B:200:ARG:HD3	1:B:384:LEU:HD11	1.87	0.56
1:A:465:ARG:HD3	1:A:545:LEU:HD11	1.88	0.56
1:A:519:ALA:O	1:A:523:ARG:HG3	2.05	0.56
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.89	0.55
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.89	0.55
1:B:465:ARG:HG3	1:B:545:LEU:HD21	1.88	0.55
1:A:227:THR:HB	1:A:347[B]:SER:O	2.07	0.54
1:B:327:ALA:O	1:B:331:GLU:HG3	2.07	0.54
1:B:172:LYS:HE3	1:B:560:ILE:HD13	1.90	0.53
1:A:148:GLN:CG	1:A:149:PRO:HD2	2.38	0.53
1:B:308:LEU:HD13	1:B:335:ALA:HB1	1.91	0.53
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.49	0.53
1:B:34:HIS:HD2	4:B:2022:HOH:O	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:CD1	1:A:335:ALA:HB1	2.39	0.52
1:A:461:GLN:HG2	1:A:541:ALA:CB	2.40	0.52
1:B:359:ASP:HB3	1:B:362:LEU:HD22	1.91	0.51
1:A:399:THR:OG1	1:A:428:HIS:HE1	1.93	0.51
1:A:545:LEU:HD13	1:A:547:LEU:HD13	1.91	0.51
1:B:268:ASN:HB3	1:B:274:CYS:SG	2.50	0.51
1:B:461:GLN:HG2	1:B:541:ALA:HB3	1.91	0.51
1:A:217:PHE:CD1	1:A:336:LEU:HD11	2.46	0.51
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.93	0.50
1:B:433:LEU:HB3	1:B:439:LEU:CD1	2.42	0.50
1:B:148:GLN:CG	1:B:149:PRO:HD2	2.41	0.50
1:B:236[B]:GLU:CD	1:B:280:ARG:HH22	2.15	0.50
1:B:523:ARG:HD3	1:B:534:LEU:HD22	1.93	0.50
1:A:268:ASN:HD21	1:A:272:GLN:NE2	2.00	0.50
1:A:52:VAL:HG22	1:A:226:SER:HG	1.72	0.49
1:B:227:THR:HB	1:B:347[B]:SER:O	2.11	0.49
1:B:18:GLU:HG3	1:B:401:ARG:NH1	2.26	0.49
1:B:361:GLU:HG3	1:B:370:VAL:O	2.14	0.48
1:A:51:LYS:HE2	4:A:2043:HOH:O	2.13	0.47
1:B:397:TRP:CE2	1:B:401:ARG:HD2	2.49	0.47
1:A:84:SER:OG	1:A:87:GLU:HG3	2.14	0.47
1:B:327:ALA:O	1:B:331:GLU:CG	2.62	0.47
1:B:433:LEU:HB3	1:B:439:LEU:HD13	1.95	0.47
1:A:313:MET:HG2	1:A:322:VAL:HB	1.97	0.47
1:A:532:THR:O	1:A:532:THR:HG23	2.15	0.47
1:A:148:GLN:HG2	1:A:149:PRO:HD2	1.96	0.47
1:A:433:LEU:HD12	1:A:438:GLN:HB2	1.97	0.46
1:B:236[B]:GLU:OE2	1:B:280:ARG:NH2	2.45	0.46
1:A:501:ARG:HE	1:A:505:ARG:NH2	2.14	0.46
1:A:416:ALA:N	1:A:417:PRO:HD2	2.31	0.46
1:A:83:LEU:HB2	1:A:173:MET:HA	1.97	0.46
1:B:331:GLU:H	1:B:331:GLU:CD	2.18	0.45
1:A:26:LEU:HB3	1:A:400:ALA:HA	1.98	0.45
1:A:423:MET:HE3	1:A:528:TRP:CZ3	2.52	0.45
1:A:26:LEU:HD23	1:A:26:LEU:O	2.16	0.45
1:B:24:ASN:HB3	1:B:27:SER:OG	2.17	0.45
1:B:11:ILE:HD13	1:B:159:LEU:HD22	1.98	0.45
1:A:27:SER:C	1:A:29:SER:N	2.70	0.44
1:B:465:ARG:HG3	1:B:545:LEU:CD2	2.47	0.44
1:B:423:MET:HA	1:B:528:TRP:CZ2	2.53	0.44
1:A:456:PRO:HA	1:A:459:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PRO:CG	1:A:400:ALA:HB1	2.48	0.44
1:A:439:LEU:O	1:A:456:PRO:HG2	2.18	0.44
1:A:27:SER:HB3	1:A:399:THR:HG21	1.99	0.44
1:B:144:VAL:HB	1:B:394:ARG:HG2	2.01	0.43
1:B:51:LYS:HE3	1:B:51:LYS:HB2	1.59	0.43
1:A:27:SER:HB2	1:A:399:THR:CG2	2.46	0.43
1:A:217:PHE:CE1	1:A:322:VAL:HG22	2.54	0.42
1:A:388:PRO:HG2	1:A:488:CYS:SG	2.60	0.42
1:B:20:LYS:HD3	1:B:20:LYS:HA	1.82	0.42
1:A:501:ARG:O	1:A:505:ARG:HG3	2.19	0.42
1:B:416:ALA:N	1:B:417:PRO:CD	2.83	0.42
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.91	0.42
1:B:347[B]:SER:C	1:B:349:PRO:HD3	2.40	0.42
1:A:148:GLN:HB3	1:A:153:GLY:HA3	2.02	0.41
1:A:532:THR:HG22	2:A:1571:SO4:S	2.60	0.41
1:B:32[B]:ARG:NH2	4:B:2039:HOH:O	2.53	0.41
1:A:434:LEU:HD12	1:A:434:LEU:HA	1.88	0.41
1:B:48[B]:ARG:HG2	1:B:159:LEU:HG	2.03	0.41
1:A:430:PHE:O	1:A:434:LEU:HB2	2.21	0.41
1:A:465:ARG:HD3	1:A:545:LEU:CD1	2.51	0.41
1:B:151:LYS:HA	1:B:151:LYS:HD3	1.34	0.41
1:B:485:VAL:O	1:B:489:LEU:HG	2.20	0.41
1:A:219:TYR:HB3	1:A:320:LEU:HD23	2.03	0.41
1:A:545:LEU:HD12	1:A:545:LEU:H	1.85	0.41
1:A:212:LYS:HB2	1:A:212:LYS:NZ	2.36	0.41
1:B:362:LEU:HD12	1:B:362:LEU:HA	1.93	0.40
1:A:46:SER:HA	1:A:49:GLN:HE21	1.86	0.40
1:A:539:ILE:HG22	1:A:541:ALA:H	1.87	0.40
1:B:200:ARG:HD3	1:B:384:LEU:CD1	2.51	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	564/579 (97%)	550 (98%)	9 (2%)	5 (1%)	17 7
1	B	569/579 (98%)	557 (98%)	10 (2%)	2 (0%)	34 24
All	All	1133/1158 (98%)	1107 (98%)	19 (2%)	7 (1%)	34 15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	543	SER
1	A	347[A]	SER
1	A	347[B]	SER
1	A	548	SER
1	A	151	LYS
1	B	347[A]	SER
1	B	347[B]	SER

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	482/493 (98%)	462 (96%)	20 (4%)	30 21
1	B	487/493 (99%)	473 (97%)	14 (3%)	42 35
All	All	969/986 (98%)	935 (96%)	34 (4%)	37 27

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	21	LEU
1	A	52	VAL
1	A	144	VAL
1	A	308	LEU
1	A	319	ASP
1	A	330	GLN
1	A	331	GLU
1	A	336	LEU

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Mol	Chain	Res	Type
1	A	362	LEU
1	A	364	THR
1	A	405	ILE
1	A	425	LEU
1	A	433	LEU
1	A	434	LEU
1	A	436	GLN
1	A	459	LEU
1	A	461	GLN
1	A	534	LEU
1	A	545	LEU
1	B	32[B]	ARG
1	B	32[D]	ARG
1	B	106	LYS
1	B	151	LYS
1	B	308	LEU
1	B	319	ASP
1	B	355	GLN
1	B	362	LEU
1	B	433	LEU
1	B	439	LEU
1	B	459	LEU
1	B	469	LEU
1	B	534	LEU
1	B	547	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	49	GLN
1	A	206	ASN
1	A	272	GLN
1	A	428	HIS
1	A	483	ASN
1	A	514	GLN
1	B	35	ASN
1	B	206	ASN

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

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 for Mogul analysis.

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	1567[B]	-	4,4,4	0.16	0	6,6,6	0.07	0
2	SO4	A	1003[B]	-	4,4,4	0.15	0	6,6,6	0.08	0
2	SO4	B	1571	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	A	1571	-	4,4,4	0.16	0	6,6,6	0.07	0
2	SO4	B	1002[B]	-	4,4,4	0.13	0	6,6,6	0.09	0
2	SO4	A	1567[A]	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	A	1003[D]	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	A	1569	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	A	1003[C]	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	A	1003[A]	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	A	1002[B]	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	A	1001	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	B	1001[B]	-	4,4,4	0.12	0	6,6,6	0.07	0
2	SO4	B	1002[C]	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	1002[D]	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	1002[A]	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	A	1570	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	B	1573	-	4,4,4	0.14	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	1002[A]	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	B	1567	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	1572	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	1569	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	B	1570	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	1001[A]	-	4,4,4	0.12	0	6,6,6	0.11	0
2	SO4	B	1003	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	B	1568	-	4,4,4	0.15	0	6,6,6	0.20	0
2	SO4	A	1568	-	4,4,4	0.15	0	6,6,6	0.08	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1571	SO4	1	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, 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	563/579 (97%)	0.42	51 (9%)	9	10	18, 41, 94, 142	0
1	B	563/579 (97%)	0.01	19 (3%)	45	48	17, 30, 62, 121	0
All	All	1126/1158 (97%)	0.21	70 (6%)	20	23	17, 35, 82, 142	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	GLY	13.2
1	A	151	LYS	11.0
1	B	542	ALA	7.6
1	B	545	LEU	7.2
1	A	534	LEU	7.0
1	B	151	LYS	6.8
1	B	153	GLY	6.8
1	A	26	LEU	6.7
1	B	152	GLY	6.5
1	A	23	ILE	6.0
1	A	149	PRO	5.5
1	A	546	ASP	4.9
1	A	150	GLU	4.9
1	A	153	GLY	4.9
1	A	532	THR	4.8
1	B	544	GLN	4.7
1	A	511	LEU	4.6
1	A	212	LYS	4.6
1	B	540	PRO	4.5
1	A	25	PRO	4.4
1	B	149	PRO	4.3
1	A	507	VAL	4.3
1	A	513	SER	4.1
1	B	543	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	523	ARG	3.9
1	A	544	GLN	3.9
1	A	548	SER	3.8
1	B	150	GLU	3.7
1	A	563	SER	3.6
1	B	15	ALA	3.6
1	A	545	LEU	3.5
1	A	509	ALA	3.4
1	A	542	ALA	3.4
1	A	213	CYS	3.3
1	A	28	ASN	3.2
1	B	539	ILE	3.2
1	A	24	ASN	3.2
1	A	531	ARG	3.1
1	B	546	ASP	3.1
1	A	535	LYS	3.1
1	B	541	ALA	3.0
1	A	148	GLN	2.9
1	B	148	GLN	2.8
1	B	534	LEU	2.8
1	A	543	SER	2.7
1	A	16	ALA	2.7
1	A	27	SER	2.7
1	A	529	ALA	2.6
1	A	15	ALA	2.6
1	A	502	HIS	2.6
1	A	434	LEU	2.5
1	A	519	ALA	2.4
1	A	537	THR	2.4
1	A	514	GLN	2.4
1	B	440	GLU	2.4
1	B	16	ALA	2.3
1	A	310	ASP	2.3
1	A	22	PRO	2.3
1	A	309	GLN	2.3
1	A	32	ARG	2.3
1	A	14	CYS	2.2
1	A	57	LEU	2.2
1	B	14	CYS	2.2
1	A	402	HIS	2.1
1	A	469	LEU	2.1
1	A	326	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	530	VAL	2.0
1	A	437	GLU	2.0
1	A	110	ASN	2.0
1	A	510	LYS	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
3	MG	A	3001	1/1	0.57	0.40	167,167,167,167	0
2	SO4	A	1570	5/5	0.74	0.26	84,88,92,92	5
2	SO4	A	1571	5/5	0.76	0.25	124,127,127,128	0
2	SO4	B	1571	5/5	0.79	0.23	28,56,59,62	5
2	SO4	B	1002[C]	5/5	0.82	0.49	43,45,46,47	5
2	SO4	B	1002[D]	5/5	0.82	0.49	34,36,46,47	5
2	SO4	B	1002[A]	5/5	0.82	0.49	29,34,40,44	5
2	SO4	B	1002[B]	5/5	0.82	0.49	20,38,43,46	5
2	SO4	B	1573	5/5	0.83	0.30	70,71,75,82	5
2	SO4	B	1572	5/5	0.83	0.20	104,106,109,114	0
2	SO4	A	1003[C]	5/5	0.84	0.55	46,46,47,53	5
2	SO4	A	1003[D]	5/5	0.84	0.55	29,34,39,41	5
2	SO4	A	1003[A]	5/5	0.84	0.55	35,36,43,48	5
2	SO4	A	1003[B]	5/5	0.84	0.55	34,43,48,48	5
2	SO4	B	1567	5/5	0.86	0.17	92,95,97,101	0
3	MG	B	3001	1/1	0.88	0.18	57,57,57,57	0
2	SO4	B	1003	5/5	0.89	0.19	103,104,106,107	0
2	SO4	B	1570	5/5	0.90	0.15	63,63,68,73	5
2	SO4	A	1569	5/5	0.90	0.16	117,119,122,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	1001	5/5	0.91	0.23	60,61,64,68	5
2	SO4	A	1567[A]	5/5	0.91	0.20	33,33,39,41	5
2	SO4	A	1567[B]	5/5	0.91	0.20	74,76,78,81	5
2	SO4	B	1001[A]	5/5	0.94	0.20	35,39,45,45	5
2	SO4	B	1001[B]	5/5	0.94	0.20	34,37,45,45	5
2	SO4	A	1002[B]	5/5	0.95	0.23	36,36,45,48	5
2	SO4	A	1002[A]	5/5	0.95	0.23	53,54,63,63	5
2	SO4	A	1568	5/5	0.96	0.15	32,48,58,60	5
2	SO4	B	1569	5/5	0.96	0.08	64,64,69,73	0
2	SO4	B	1568	5/5	0.98	0.07	42,42,44,55	0

6.5 Other polymers (i)

There are no such residues in this entry.