



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:55 PM GMT

PDB ID : 4GMC
Title : Crystal structure of HCV NS5B polymerase in complex with a thumb inhibitor
Authors : Coulombe, R.
Deposited on : 2012-08-15
Resolution : 2.70 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

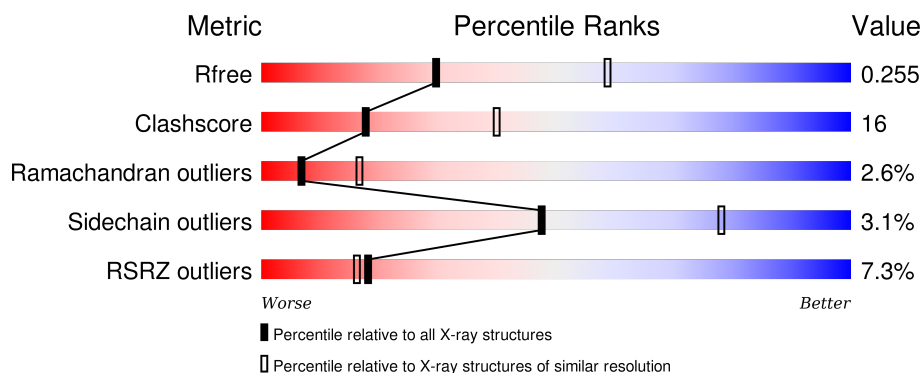
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	576	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 72% 23% • • </div> </div>
1	B	576	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 13% 57% 32% 5% • 6% </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	603	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8692 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.

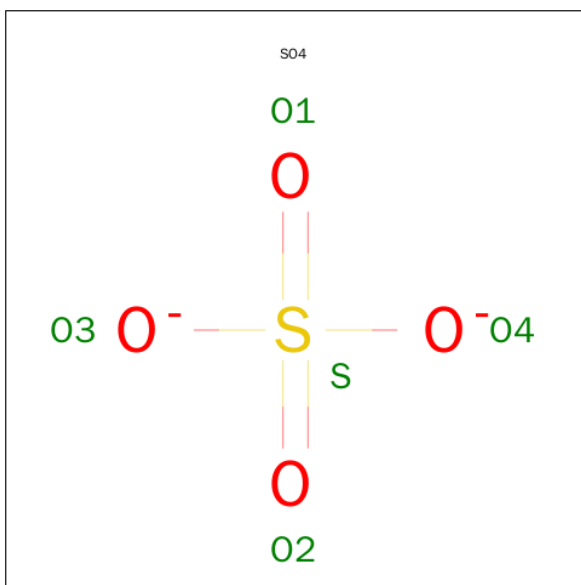
- Molecule 1 is a protein called NS5B polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4358	2745	770	811	32			
1	B	541	Total	C	N	O	S	0	0	0
			4210	2652	741	785	32			

There are 12 discrepancies between the modelled and reference sequences:

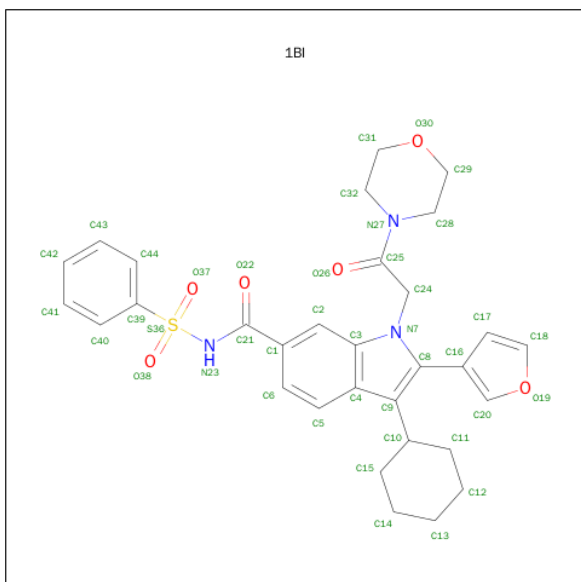
Chain	Residue	Modelled	Actual	Comment	Reference
A	571	HIS	-	EXPRESSION TAG	UNP O92972
A	572	HIS	-	EXPRESSION TAG	UNP O92972
A	573	HIS	-	EXPRESSION TAG	UNP O92972
A	574	HIS	-	EXPRESSION TAG	UNP O92972
A	575	HIS	-	EXPRESSION TAG	UNP O92972
A	576	HIS	-	EXPRESSION TAG	UNP O92972
B	571	HIS	-	EXPRESSION TAG	UNP O92972
B	572	HIS	-	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

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

- Molecule 3 is 3-CYCLOHEXYL-2-(FURAN-3-YL)-1-[2-(MORPHOLIN-4-YL)-2-OXOETHYL]-N-(PHENYLSULFONYL)-1H-INDOLE-6-CARBOXAMIDE (three-letter code: 1BI) (formula: C₃₁H₃₃N₃O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			41	31	3	6	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	21	Total	O	0	0
			21	21		

R498	T499	W500	R501	H502	R503	A504	R505	S506	V507	R508		L511	L512	S513	Q514	G515	G516	R517	A518	A519	T520	C521	G522	R523	T524	L525	F526	N527	N528	A529	V530	R531	K533	T532	L534	K535	L536	T537	P538	I539	P540	A541	A542	S543	Q544	L545	D546	L547	S548	G549	F551	V552		D559	I560	Y561	H562	S563																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.24Å 106.26Å 133.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 49.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.70) 99.7 (49.65-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.257 0.218 , 0.255	Depositor DCC
R_{free} test set	4127 reflections (9.99%)	DCC
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.8	EDS
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 46323 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8692	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: 1BI, 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	0.38	0/4453	0.63	1/6044 (0.0%)
1	B	0.39	0/4299	0.71	3/5831 (0.1%)
All	All	0.38	0/8752	0.67	4/11875 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	516	GLY	N-CA-C	-11.62	84.06	113.10
1	A	351	GLY	N-CA-C	-5.67	98.92	113.10
1	B	402	HIS	N-CA-C	5.45	125.72	111.00
1	B	11	ILE	N-CA-C	-5.05	97.36	111.00

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	4358	0	4371	91	0
1	B	4210	0	4218	187	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
3	B	41	0	33	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	42	0	0	1	0
4	B	21	0	0	1	0
All	All	8692	0	8622	275	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 (275) 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:536:LEU:HD12	1:B:536:LEU:H	1.14	1.10
1:B:405:ILE:HG21	1:B:443:LEU:HD13	1.43	1.00
1:B:13:PRO:HB3	1:B:17:GLU:HB2	1.45	0.97
1:B:434:LEU:HD23	1:B:434:LEU:H	1.38	0.89
1:B:514:GLN:HG2	1:B:515:GLY:N	1.85	0.88
1:B:514:GLN:HG2	1:B:515:GLY:H	1.36	0.88
1:B:434:LEU:HD22	1:B:511:LEU:HD21	1.55	0.87
1:B:37:VAL:HG21	3:B:601:1BI:H16	1.58	0.85
1:B:523:ARG:HG3	1:B:534:LEU:HD23	1.61	0.82
1:B:464:GLU:O	1:B:468:GLY:HA2	1.81	0.81
1:A:523:ARG:HG3	1:A:534:LEU:HD12	1.62	0.80
1:B:536:LEU:HD12	1:B:536:LEU:N	1.94	0.78
1:B:508:ARG:HH12	1:B:530:VAL:HG21	1.49	0.77
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.68	0.75
1:B:499:THR:O	1:B:503:ARG:HG3	1.87	0.74
1:B:547:LEU:HA	1:B:550:TRP:NE1	2.05	0.71
1:B:147:VAL:HG11	1:B:154:ARG:HH21	1.56	0.70
1:B:405:ILE:O	1:B:405:ILE:HG22	1.90	0.70
1:B:403:THR:O	1:B:404:PRO:C	2.29	0.70
1:B:424:ILE:HD13	1:B:489:LEU:HD21	1.73	0.69
1:B:423:MET:HA	1:B:528:TRP:CZ2	2.28	0.69
1:B:118:HIS:O	1:B:121:SER:HB3	1.93	0.68
1:B:13:PRO:CB	1:B:17:GLU:HB2	2.22	0.68
1:B:196:SER:OG	1:B:199:GLN:HG3	1.94	0.68
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.75	0.68
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.75	0.68
1:B:403:THR:OG1	1:B:404:PRO:HD2	1.93	0.67
1:B:138:ILE:O	1:B:139:MET:HG2	1.95	0.67
1:A:545:LEU:HD13	1:A:547:LEU:HD11	1.74	0.67
1:B:493:GLY:O	3:B:601:1BI:H20	1.95	0.67
1:B:465:ARG:NH1	1:B:545:LEU:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:VAL:HG12	1:B:373:ALA:H	1.60	0.66
1:B:359:ASP:HB3	1:B:362:LEU:HD12	1.78	0.65
1:B:536:LEU:CD1	1:B:536:LEU:H	1.93	0.65
1:B:514:GLN:CG	1:B:515:GLY:H	2.01	0.65
1:A:248:GLU:HG3	4:A:717:HOH:O	1.96	0.64
1:B:447:ILE:HD12	1:B:550:TRP:HZ3	1.62	0.64
1:B:547:LEU:HA	1:B:550:TRP:HE1	1.61	0.64
1:A:346:TYR:O	1:A:347:SER:HB3	1.97	0.63
1:A:308:LEU:CD1	1:A:335:ALA:HB1	2.28	0.63
1:B:462:ILE:HA	1:B:545:LEU:CD1	2.28	0.63
1:B:99:SER:HB2	1:B:165:LEU:HB3	1.80	0.63
1:B:478:SER:O	1:B:482:ILE:HG13	1.99	0.63
1:A:313:MET:HG2	1:A:322:VAL:HG22	1.81	0.62
1:B:13:PRO:O	1:B:14:CYS:HB2	1.98	0.62
1:B:138:ILE:HD11	1:B:159:LEU:HD13	1.82	0.62
1:B:454:ILE:HG22	1:B:455:GLU:N	2.14	0.62
1:A:254:ARG:HG2	1:B:251:GLN:NE2	2.15	0.62
1:B:470:SER:O	1:B:474:LEU:HG	1.99	0.61
1:B:405:ILE:HG13	1:B:443:LEU:HD22	1.80	0.61
1:B:248:GLU:HG3	4:B:705:HOH:O	2.00	0.61
1:B:327:ALA:HB1	1:B:331:GLU:OE1	2.00	0.61
1:B:147:VAL:CG1	1:B:154:ARG:HH21	2.14	0.60
1:B:383:TYR:HH	1:B:477:TYR:HD2	1.50	0.60
1:A:439:LEU:O	1:A:457:LEU:HG	2.01	0.60
1:A:466:LEU:HD22	1:A:551:PHE:HE2	1.66	0.60
1:B:40:THR:HB	1:B:157:ALA:HB2	1.84	0.60
1:B:15:ALA:O	1:B:16:ALA:HB3	2.02	0.60
1:B:13:PRO:HG3	1:B:42:SER:OG	2.02	0.59
1:B:386:ARG:NH2	1:B:391:PRO:HD3	2.17	0.59
1:B:93:PRO:HG3	1:B:561:TYR:HB2	1.85	0.59
1:B:129:ASP:HB3	1:B:259:ARG:NH1	2.18	0.58
1:B:508:ARG:NH1	1:B:530:VAL:HG11	2.18	0.58
1:B:364:THR:HA	1:B:368:SER:O	2.04	0.58
1:A:331:GLU:H	1:A:331:GLU:CD	2.06	0.58
1:B:452:TYR:O	1:B:453:SER:HB2	2.04	0.58
1:B:5:THR:O	1:B:275:GLY:HA3	2.04	0.57
1:A:5:THR:O	1:A:275:GLY:HA3	2.03	0.57
1:B:336:LEU:CD2	1:B:356:PRO:HD3	2.35	0.56
1:B:532:THR:O	1:B:533:LYS:HB2	2.04	0.56
1:B:85:ILE:HD11	1:B:120:ARG:HG2	1.86	0.56
1:A:21:LEU:HD12	1:A:22:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:PHE:O	1:B:433:LEU:HB2	2.06	0.56
1:A:436:GLN:O	1:A:438:GLN:HG3	2.05	0.56
1:B:83:LEU:HB2	1:B:173:MET:HA	1.88	0.56
1:A:93:PRO:HG3	1:A:561:TYR:HB2	1.87	0.56
1:A:40:THR:HB	1:A:157:ALA:HB2	1.88	0.56
1:B:109:ARG:HH11	1:B:109:ARG:HG2	1.70	0.56
1:B:424:ILE:CD1	1:B:489:LEU:HD21	2.35	0.56
1:B:459:LEU:HB2	1:B:460:PRO:HD3	1.88	0.56
1:B:433:LEU:HD13	1:B:439:LEU:HD23	1.87	0.55
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.88	0.55
1:B:421:ALA:O	1:B:426:MET:HG3	2.06	0.55
1:B:461:GLN:HG2	1:B:541:ALA:HB3	1.88	0.55
1:B:408:TRP:O	1:B:412:ILE:HG13	2.06	0.55
1:A:368:SER:HB3	1:A:384:LEU:HG	1.87	0.55
1:B:481:GLU:O	1:B:485:VAL:HG23	2.06	0.55
1:A:268:ASN:HD21	1:A:272:GLN:HB2	1.71	0.55
1:A:234:ARG:NH1	1:A:258:GLU:OE2	2.39	0.55
1:A:33:HIS:HB2	1:A:492:LEU:O	2.07	0.55
1:B:85:ILE:CD1	1:B:120:ARG:HG2	2.37	0.54
1:B:46:SER:HA	1:B:49:GLN:NE2	2.22	0.54
1:B:46:SER:HA	1:B:49:GLN:HE21	1.72	0.54
1:B:404:PRO:HB3	1:B:406:ASN:HD21	1.72	0.54
1:A:515:GLY:CA	1:A:519:ALA:HB2	2.36	0.54
1:B:372:VAL:HG12	1:B:373:ALA:N	2.22	0.54
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.89	0.54
1:B:423:MET:HG2	1:B:528:TRP:CZ3	2.43	0.54
1:B:376:ALA:O	1:B:377:SER:C	2.46	0.54
1:B:15:ALA:O	1:B:16:ALA:CB	2.56	0.54
1:B:438:GLN:C	1:B:440:GLU:H	2.10	0.53
1:B:447:ILE:HD12	1:B:550:TRP:CZ3	2.43	0.53
1:A:13:PRO:HG3	1:A:42:SER:OG	2.09	0.53
1:A:542:ALA:O	1:A:545:LEU:HB2	2.08	0.53
1:B:454:ILE:HG22	1:B:455:GLU:H	1.74	0.52
1:B:542:ALA:H	1:B:544:GLN:H	1.58	0.52
1:B:469:LEU:N	1:B:469:LEU:HD23	2.25	0.52
1:B:336:LEU:HD23	1:B:356:PRO:HD3	1.91	0.52
1:A:254:ARG:HG2	1:B:251:GLN:HE22	1.75	0.52
1:B:416:ALA:HB3	1:B:467:HIS:CD2	2.44	0.52
1:A:308:LEU:HD12	1:A:335:ALA:HB1	1.92	0.51
1:A:83:LEU:HB2	1:A:173:MET:HA	1.91	0.51
1:A:547:LEU:O	1:A:550:TRP:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:THR:HB	1:A:391:PRO:HD3	1.91	0.51
1:A:57:LEU:C	1:A:57:LEU:HD23	2.31	0.51
1:A:336:LEU:HD21	1:A:354:PRO:HB2	1.93	0.51
1:A:18:GLU:HG3	1:A:401:ARG:NH1	2.26	0.51
1:A:134:ILE:HG13	1:A:259:ARG:HB3	1.92	0.51
1:B:309:GLN:O	1:B:324:CYS:HB2	2.10	0.51
1:A:233:ILE:HD13	1:A:261:TYR:O	2.11	0.51
1:B:187:MET:HE3	1:B:296:TYR:HB2	1.93	0.50
1:B:222:ARG:HG2	1:B:222:ARG:HH11	1.76	0.50
1:A:69:LYS:HE2	1:B:77:THR:O	2.11	0.50
1:A:182:LEU:HD12	1:A:243:CYS:SG	2.52	0.50
1:A:523:ARG:HH11	1:A:534:LEU:CD1	2.24	0.50
1:B:170:CYS:HA	1:B:173:MET:CE	2.41	0.50
1:B:501:ARG:HH11	1:B:501:ARG:HG3	1.77	0.49
1:B:285:LEU:HD11	1:B:560:ILE:HD11	1.94	0.49
1:A:309:GLN:O	1:A:324:CYS:HB2	2.11	0.49
1:A:64:TYR:CZ	1:A:297:LEU:HD21	2.47	0.49
1:A:191:TYR:O	1:A:194:GLN:HG2	2.13	0.49
1:B:438:GLN:C	1:B:440:GLU:N	2.65	0.49
1:B:547:LEU:HA	1:B:550:TRP:CD1	2.48	0.49
1:B:403:THR:CB	1:B:404:PRO:CD	2.91	0.49
1:A:183:PRO:HG3	1:A:289:CYS:SG	2.52	0.49
1:B:170:CYS:HA	1:B:173:MET:HE3	1.95	0.49
1:A:308:LEU:HD11	1:A:335:ALA:HB1	1.93	0.49
1:A:86:GLU:HG3	1:A:111:LEU:HD11	1.94	0.48
1:B:413:ILE:HD13	1:B:454:ILE:HD12	1.95	0.48
1:B:346:TYR:O	1:B:347:SER:HB3	2.13	0.48
1:B:508:ARG:O	1:B:512:LEU:HB2	2.13	0.48
1:B:13:PRO:O	1:B:14:CYS:CB	2.62	0.48
1:B:455:GLU:HB2	1:B:458:ASP:OD2	2.13	0.48
1:A:268:ASN:ND2	1:A:272:GLN:HB2	2.28	0.48
1:A:86:GLU:CG	1:A:111:LEU:HD11	2.43	0.48
1:B:264:GLY:HA2	1:B:276:TYR:CZ	2.48	0.48
1:A:426:MET:SD	1:A:525:LEU:HD22	2.53	0.48
1:B:501:ARG:O	1:B:505:ARG:HG3	2.13	0.48
1:A:531:ARG:HD3	1:A:531:ARG:HA	1.62	0.47
1:B:187:MET:HE2	1:B:296:TYR:CD2	2.48	0.47
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.95	0.47
1:B:423:MET:HE1	1:B:497:LEU:HB3	1.95	0.47
1:B:388:PRO:C	1:B:391:PRO:HD2	2.34	0.47
1:B:134:ILE:HG13	1:B:259:ARG:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:THR:O	1:B:538:PRO:C	2.53	0.47
1:B:109:ARG:HG2	1:B:109:ARG:NH1	2.29	0.47
1:B:503:ARG:O	1:B:507:VAL:HG23	2.14	0.47
1:A:306:ALA:O	1:A:307:LYS:HB2	2.14	0.47
1:B:321:VAL:O	1:B:321:VAL:HG13	2.13	0.47
1:A:30:LEU:O	1:A:494:VAL:HG13	2.14	0.47
1:B:508:ARG:HH12	1:B:530:VAL:CG2	2.25	0.46
1:B:390:THR:HB	1:B:391:PRO:HD3	1.97	0.46
1:A:83:LEU:HD22	1:A:176:TYR:HB3	1.97	0.46
1:A:196:SER:OG	1:A:199:GLN:HG3	2.16	0.46
1:A:523:ARG:HG3	1:A:534:LEU:CD1	2.41	0.46
1:B:367:SER:O	1:B:386:ARG:HB3	2.15	0.46
1:B:416:ALA:HB3	1:B:417:PRO:HD3	1.98	0.46
1:B:465:ARG:CD	1:B:547:LEU:HD22	2.45	0.46
1:A:308:LEU:HB3	1:A:311:CYS:SG	2.56	0.46
1:B:96:SER:HB3	1:B:105:ALA:HB2	1.98	0.46
1:A:116:VAL:O	1:A:120:ARG:HG2	2.16	0.46
1:B:398:GLU:CD	1:B:407:SER:HG	2.18	0.46
1:B:462:ILE:HA	1:B:545:LEU:HD13	1.98	0.46
1:B:547:LEU:HG	1:B:550:TRP:CD1	2.50	0.46
1:B:431:SER:O	1:B:435:ALA:HB2	2.16	0.46
1:B:465:ARG:HH11	1:B:545:LEU:HB2	1.81	0.45
1:A:158:ARG:NH2	2:A:601:SO4:O2	2.49	0.45
1:B:505:ARG:NH2	1:B:530:VAL:HG12	2.31	0.45
1:B:462:ILE:HA	1:B:545:LEU:HD11	1.96	0.45
1:B:545:LEU:HA	1:B:545:LEU:HD23	1.54	0.45
1:A:331:GLU:N	1:A:331:GLU:CD	2.70	0.45
1:A:36:MET:O	1:A:146:CYS:HA	2.16	0.45
1:B:495:PRO:HB3	1:B:499:THR:CB	2.47	0.45
1:B:532:THR:O	1:B:533:LYS:CB	2.65	0.45
1:B:215:MET:HB2	1:B:326:SER:HB2	1.99	0.45
1:A:313:MET:CG	1:A:322:VAL:HG22	2.45	0.45
1:B:38:TYR:CZ	1:B:145:PHE:HB2	2.52	0.45
1:A:375:ASP:OD2	1:A:379:LYS:HB3	2.17	0.45
1:B:454:ILE:CG2	1:B:455:GLU:N	2.80	0.44
1:A:203:PHE:CE2	1:A:314:LEU:HD13	2.51	0.44
1:A:32:ARG:HD2	1:A:32:ARG:N	2.32	0.44
1:A:434:LEU:HD21	1:A:511:LEU:HD23	2.00	0.44
1:B:546:ASP:O	1:B:548:SER:N	2.44	0.44
1:B:141:LYS:HG2	1:B:142:SER:N	2.33	0.44
1:B:357:GLU:HG3	1:B:362:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:THR:O	1:B:539:ILE:N	2.50	0.44
1:B:73:ALA:O	1:B:76:SER:HB2	2.17	0.44
1:A:122:VAL:HG12	1:A:170:CYS:SG	2.58	0.44
1:A:42:SER:HA	1:A:140:ALA:CB	2.48	0.44
1:B:418:THR:O	1:B:422:ARG:HG3	2.17	0.44
1:B:443:LEU:O	1:B:453:SER:HA	2.18	0.44
1:B:432:ILE:HG22	1:B:432:ILE:O	2.17	0.43
1:A:223:CYS:O	1:A:227:THR:HG23	2.18	0.43
1:B:222:ARG:NH1	1:B:222:ARG:HG2	2.33	0.43
1:B:433:LEU:C	1:B:435:ALA:N	2.71	0.43
1:B:175:LEU:HD21	1:B:253:ILE:HG12	2.00	0.43
1:B:92:THR:O	1:B:109:ARG:NH1	2.52	0.43
1:B:107:ASP:HB3	1:B:112:SER:OG	2.18	0.43
1:A:523:ARG:HH11	1:A:534:LEU:HD13	1.83	0.43
1:B:215:MET:SD	1:B:215:MET:C	2.96	0.43
1:B:437:GLU:O	1:B:437:GLU:HG3	2.19	0.43
1:B:495:PRO:HB3	1:B:499:THR:HB	1.99	0.43
1:B:328:GLY:O	1:B:329:THR:C	2.57	0.43
1:B:220:ASP:OD2	1:B:351:GLY:HA3	2.19	0.43
1:B:442:ALA:HB2	1:B:455:GLU:HG2	2.01	0.43
1:B:501:ARG:NH1	1:B:501:ARG:HG3	2.34	0.43
1:B:93:PRO:HD3	1:B:559:ASP:O	2.19	0.43
1:A:555:TYR:CD1	1:A:560:ILE:HG13	2.53	0.43
1:A:84:SER:OG	1:A:87:GLU:HG3	2.19	0.43
1:B:201:VAL:HG22	1:B:384:LEU:HD13	2.00	0.43
1:B:212:LYS:HB2	1:B:325:GLU:OE2	2.19	0.43
1:B:409:LEU:O	1:B:413:ILE:HG13	2.18	0.43
1:A:309:GLN:CA	1:A:309:GLN:HE21	2.31	0.43
1:B:403:THR:CB	1:B:404:PRO:HD2	2.49	0.42
1:B:470:SER:C	1:B:472:PHE:H	2.22	0.42
1:A:26:LEU:HD12	1:A:26:LEU:HA	1.86	0.42
1:A:314:LEU:HA	1:A:314:LEU:HD12	1.92	0.42
1:B:441:LYS:HD3	1:B:443:LEU:HD21	2.01	0.42
1:B:139:MET:HB2	1:B:160:ILE:CG1	2.50	0.42
1:A:215:MET:HG3	1:A:332:ASP:OD2	2.20	0.42
1:B:515:GLY:HA3	1:B:518:ALA:HB3	2.01	0.42
1:A:428:HIS:O	1:A:431:SER:HB3	2.19	0.42
1:B:508:ARG:NH1	1:B:530:VAL:HG21	2.27	0.42
1:B:407:SER:O	1:B:408:TRP:C	2.57	0.42
1:B:530:VAL:C	1:B:532:THR:H	2.22	0.42
1:B:394:ARG:O	1:B:398:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PRO:HD3	1:A:559:ASP:O	2.19	0.42
1:B:208:TRP:NE1	1:B:214:PRO:HG3	2.35	0.42
1:A:544:GLN:O	1:A:544:GLN:HG2	2.19	0.42
1:B:39:ALA:HA	1:B:143:GLU:O	2.19	0.42
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.79	0.42
1:B:309:GLN:O	1:B:310:ASP:C	2.58	0.42
1:B:405:ILE:CG2	1:B:405:ILE:O	2.62	0.41
1:A:561:TYR:O	1:A:561:TYR:CD2	2.73	0.41
1:A:422:ARG:O	1:A:426:MET:HB2	2.20	0.41
1:B:479:PRO:O	1:B:483:ASN:ND2	2.53	0.41
1:B:426:MET:O	1:B:430:PHE:HB2	2.20	0.41
1:B:461:GLN:HB3	1:B:541:ALA:O	2.20	0.41
1:B:191:TYR:O	1:B:194:GLN:HG2	2.21	0.41
1:A:21:LEU:HD23	1:A:34:HIS:HA	2.01	0.41
1:B:444:ASP:HA	1:B:453:SER:HA	2.02	0.41
1:A:440:GLU:HG2	1:A:457:LEU:HD12	2.03	0.41
1:B:433:LEU:O	1:B:436:GLN:N	2.51	0.41
1:B:138:ILE:C	1:B:139:MET:HG2	2.41	0.41
1:B:298:LYS:HE2	1:B:346:TYR:O	2.20	0.41
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.94	0.41
1:A:479:PRO:O	1:A:483:ASN:OD1	2.39	0.41
1:B:48:ARG:HD3	1:B:52:VAL:HG13	2.03	0.41
1:B:547:LEU:O	1:B:548:SER:O	2.39	0.41
1:B:489:LEU:HD22	1:B:494:VAL:HB	2.03	0.41
1:A:219:TYR:HB3	1:A:320:LEU:HD23	2.03	0.41
1:A:458:ASP:OD1	1:A:517:ARG:NH1	2.54	0.41
1:A:406:ASN:ND2	1:A:443:LEU:HB3	2.36	0.41
1:B:386:ARG:HH21	1:B:391:PRO:HD3	1.83	0.40
1:A:81:LYS:HG2	1:A:177:ASP:OD2	2.21	0.40
1:B:454:ILE:CG2	1:B:455:GLU:H	2.34	0.40
1:A:21:LEU:HA	1:A:22:PRO:HD3	1.94	0.40
1:B:414:MET:O	1:B:467:HIS:HE1	2.04	0.40
1:A:45:ALA:O	1:A:49:GLN:HG3	2.21	0.40
1:A:416:ALA:N	1:A:417:PRO:CD	2.84	0.40
1:B:359:ASP:CB	1:B:362:LEU:HD12	2.49	0.40
1:B:440:GLU:O	1:B:441:LYS:C	2.59	0.40
1:B:138:ILE:HB	1:B:266:LEU:HD22	2.03	0.40
1:A:226:SER:HA	1:A:279:CYS:SG	2.62	0.40
1:B:306:ALA:O	1:B:307:LYS:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	555/576 (96%)	521 (94%)	31 (6%)	3 (0%)	34	63
1	B	535/576 (93%)	457 (85%)	53 (10%)	25 (5%)	3	5
All	All	1090/1152 (95%)	978 (90%)	84 (8%)	28 (3%)	7	16

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	14	CYS
1	B	16	ALA
1	B	329	THR
1	B	403	THR
1	B	404	PRO
1	B	406	ASN
1	B	407	SER
1	B	453	SER
1	B	534	LEU
1	B	540	PRO
1	B	542	ALA
1	B	548	SER
1	B	13	PRO
1	B	376	ALA
1	B	468	GLY
1	B	469	LEU
1	B	515	GLY
1	B	533	LYS
1	A	347	SER
1	B	470	SER
1	B	514	GLN
1	B	538	PRO
1	A	541	ALA
1	B	193	PHE
1	B	310	ASP

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Mol	Chain	Res	Type
1	B	441	LYS
1	B	541	ALA
1	A	540	PRO

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	477/491 (97%)	461 (97%)	16 (3%)	44	75
1	B	458/491 (93%)	445 (97%)	13 (3%)	51	81
All	All	935/982 (95%)	906 (97%)	29 (3%)	47	78

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

Mol	Chain	Res	Type
1	A	26	LEU
1	A	50	LYS
1	A	57	LEU
1	A	86	GLU
1	A	106	LYS
1	A	112	SER
1	A	159	LEU
1	A	273	ASN
1	A	308	LEU
1	A	309	GLN
1	A	336	LEU
1	A	402	HIS
1	A	446	GLN
1	A	474	LEU
1	A	492	LEU
1	A	545	LEU
1	B	41	THR
1	B	139	MET
1	B	273	ASN
1	B	383	TYR

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Mol	Chain	Res	Type
1	B	401	ARG
1	B	402	HIS
1	B	404	PRO
1	B	406	ASN
1	B	434	LEU
1	B	469	LEU
1	B	536	LEU
1	B	539	ILE
1	B	546	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	273	ASN
1	A	309	GLN
1	A	406	ASN
1	A	483	ASN
1	A	544	GLN
1	B	49	GLN
1	B	206	ASN
1	B	251	GLN
1	B	273	ASN
1	B	406	ASN
1	B	436	GLN
1	B	446	GLN
1	B	483	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 carbohydrates in this entry.

5.6 Ligand geometry

5 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	601	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	A	602	-	4,4,4	0.18	0	6,6,6	0.18	0
3	1BI	B	601	-	40,46,46	3.63	24 (60%)	49,66,66	2.27	8 (16%)
2	SO4	B	602	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	B	603	-	4,4,4	0.25	0	6,6,6	0.11	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	601	-	-	0/0/0/0	0/0/0/0
2	SO4	A	602	-	-	0/0/0/0	0/0/0/0
3	1BI	B	601	-	-	0/23/47/47	0/5/6/6
2	SO4	B	602	-	-	0/0/0/0	0/0/0/0
2	SO4	B	603	-	-	0/0/0/0	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	1BI	O37-S36	-6.20	1.36	1.43
3	B	601	1BI	O38-S36	-5.42	1.37	1.43
3	B	601	1BI	S36-N23	-4.78	1.54	1.64
3	B	601	1BI	C41-C40	2.18	1.43	1.38
3	B	601	1BI	C15-C10	2.27	1.59	1.53
3	B	601	1BI	C32-N27	2.34	1.51	1.47
3	B	601	1BI	C43-C44	2.38	1.43	1.38
3	B	601	1BI	C41-C42	2.52	1.44	1.38
3	B	601	1BI	C42-C43	2.68	1.44	1.38
3	B	601	1BI	C2-C3	2.94	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	1BI	C5-C4	3.12	1.48	1.42
3	B	601	1BI	C40-C39	3.15	1.44	1.38
3	B	601	1BI	C44-C39	3.35	1.44	1.38
3	B	601	1BI	O30-C29	3.76	1.58	1.42
3	B	601	1BI	O30-C31	3.77	1.58	1.42
3	B	601	1BI	C6-C1	3.82	1.45	1.39
3	B	601	1BI	C28-N27	3.91	1.53	1.47
3	B	601	1BI	C39-S36	4.09	1.82	1.76
3	B	601	1BI	C5-C6	4.13	1.45	1.36
3	B	601	1BI	C24-C25	5.44	1.58	1.52
3	B	601	1BI	C25-N27	5.54	1.47	1.35
3	B	601	1BI	C2-C1	6.08	1.47	1.37
3	B	601	1BI	C9-C4	6.20	1.47	1.40
3	B	601	1BI	C21-N23	10.11	1.50	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	1BI	C1-C21-N23	-8.34	106.51	116.05
3	B	601	1BI	O37-S36-O38	-6.98	110.28	119.54
3	B	601	1BI	C21-N23-S36	-4.26	118.34	123.33
3	B	601	1BI	C24-C25-N27	2.35	120.45	117.02
3	B	601	1BI	C28-N27-C32	3.34	118.75	112.56
3	B	601	1BI	O22-C21-C1	3.40	126.78	120.97
3	B	601	1BI	C25-C24-N7	4.28	115.72	110.82
3	B	601	1BI	O22-C21-N23	6.38	126.70	120.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	SO4	1	0
3	B	601	1BI	2	0

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

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	559/576 (97%)	-0.07	5 (0%) 85 86	23, 38, 63, 91	0
1	B	541/576 (93%)	0.64	75 (13%) 4 3	22, 58, 109, 119	0
All	All	1100/1152 (95%)	0.28	80 (7%) 18 16	22, 43, 101, 119	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	511	LEU	7.3
1	B	524	TYR	6.7
1	B	542	ALA	6.3
1	B	534	LEU	5.9
1	B	518	ALA	5.6
1	B	516	GLY	5.5
1	B	520	THR	5.2
1	B	530	VAL	5.0
1	B	15	ALA	4.9
1	B	535	LYS	4.7
1	B	512	LEU	4.6
1	B	531	ARG	4.6
1	B	16	ALA	4.5
1	B	519	ALA	4.5
1	B	523	ARG	4.5
1	B	541	ALA	4.5
1	B	532	THR	4.4
1	B	549	GLY	4.4
1	B	515	GLY	4.4
1	B	536	LEU	4.2
1	B	405	ILE	4.0
1	B	17	GLU	4.0
1	B	14	CYS	4.0
1	B	533	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	472	PHE	3.8
1	B	529	ALA	3.7
1	B	469	LEU	3.7
1	B	547	LEU	3.7
1	B	526	PHE	3.5
1	B	539	ILE	3.5
1	B	525	LEU	3.4
1	B	545	LEU	3.4
1	B	331	GLU	3.4
1	B	442	ALA	3.4
1	B	381	VAL	3.2
1	B	538	PRO	3.2
1	B	537	THR	3.2
1	B	402	HIS	3.2
1	B	521	CYS	3.1
1	B	471	ALA	3.1
1	B	528	TRP	3.0
1	B	437	GLU	3.0
1	B	212	LYS	3.0
1	B	466	LEU	3.0
1	B	213	CYS	3.0
1	B	507	VAL	2.9
1	B	544	GLN	2.9
1	B	465	ARG	2.9
1	A	539	ILE	2.9
1	B	548	SER	2.9
1	B	513	SER	2.8
1	B	208	TRP	2.8
1	B	377	SER	2.7
1	B	552	VAL	2.7
1	A	544	GLN	2.7
1	B	514	GLN	2.7
1	B	517	ARG	2.6
1	A	543	SER	2.6
1	B	459	LEU	2.6
1	B	373	ALA	2.6
1	B	153	GLY	2.6
1	B	455	GLU	2.6
1	B	468	GLY	2.6
1	B	453	SER	2.5
1	B	563	SER	2.5
1	B	440	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	561	TYR	2.5
1	B	438	GLN	2.5
1	A	542	ALA	2.4
1	B	508	ARG	2.3
1	B	504	ALA	2.2
1	B	214	PRO	2.2
1	B	454	ILE	2.2
1	B	324	CYS	2.2
1	B	439	LEU	2.2
1	A	540	PRO	2.1
1	B	13	PRO	2.1
1	B	335	ALA	2.1
1	B	464	GLU	2.1
1	B	461	GLN	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	B	603	5/5	0.88	0.31	6.06	103,103,104,104	0
2	SO4	A	601	5/5	0.92	0.21	1.53	95,95,95,96	0
2	SO4	A	602	5/5	0.95	0.20	1.33	74,75,75,76	0
3	1BI	B	601	41/41	0.87	0.21	1.14	64,73,83,85	0
2	SO4	B	602	5/5	0.92	0.21	0.96	104,104,105,105	0

6.5 Other polymers

There are no such residues in this entry.