



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:20 pm BST

PDB ID : 1RP5  
Title : PBP2x from Streptococcus pneumoniae strain 5259 with reduced susceptibility to beta-lactam antibiotics  
Authors : Pernot, L.; Chesnel, L.; Legouellec, A.; Croize, J.; Vernet, T.; Dideberg, O.; Dessen, A.  
Deposited on : 2003-12-03  
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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

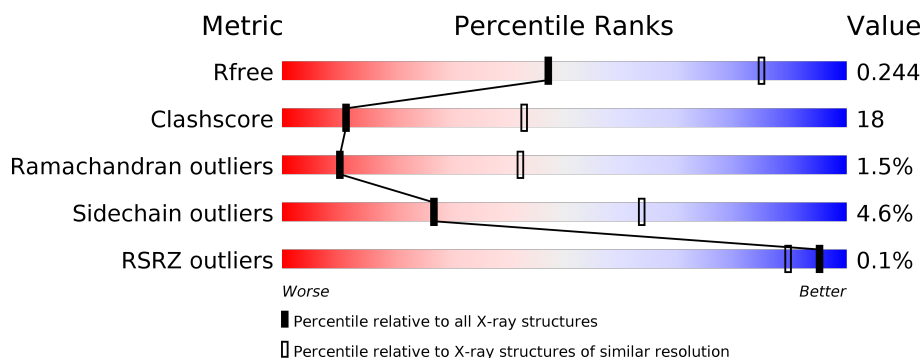
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	702	 66% 29% . .
1	B	702	 65% 29% . .

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	A	751	-	-	X	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10315 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 penicillin-binding protein 2x.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	S	0	0	0
			5128	3219	851	1034	24			
1	B	680	Total	C	N	O	S	0	0	0
			5132	3219	853	1036	24			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

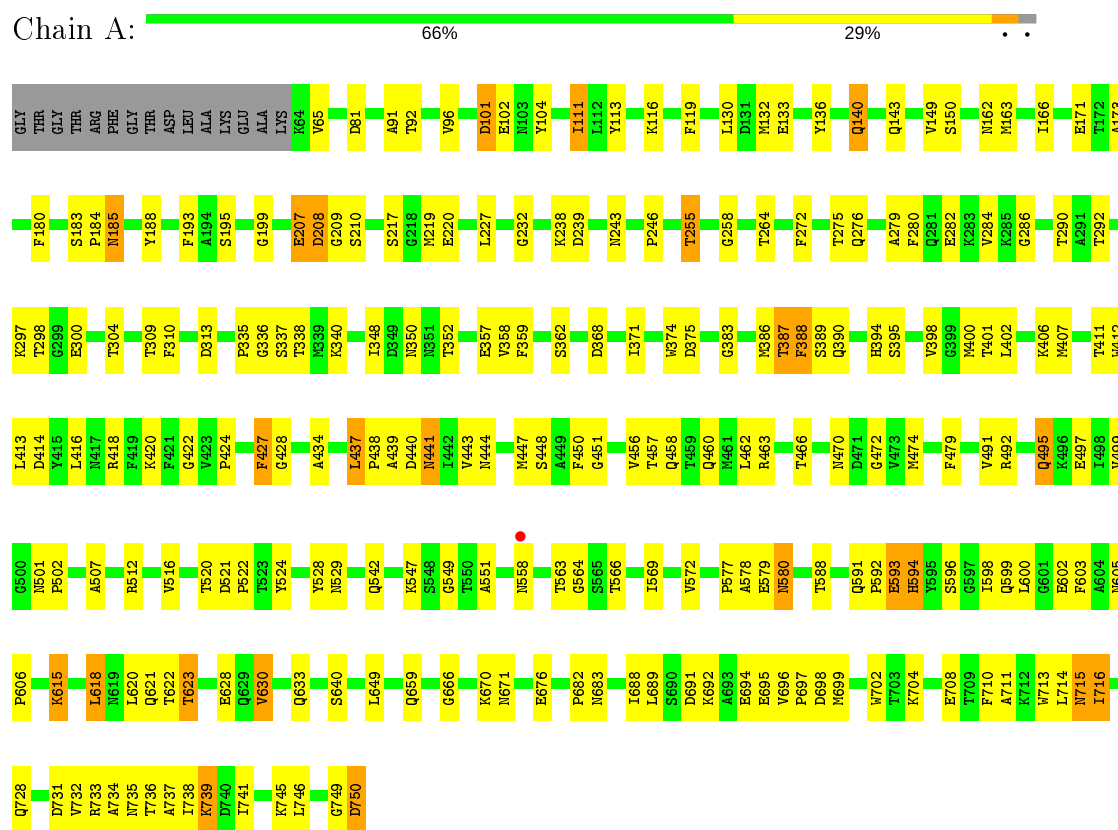
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total 19	O 19	0	0
3	B	26	Total 26	O 26	0	0

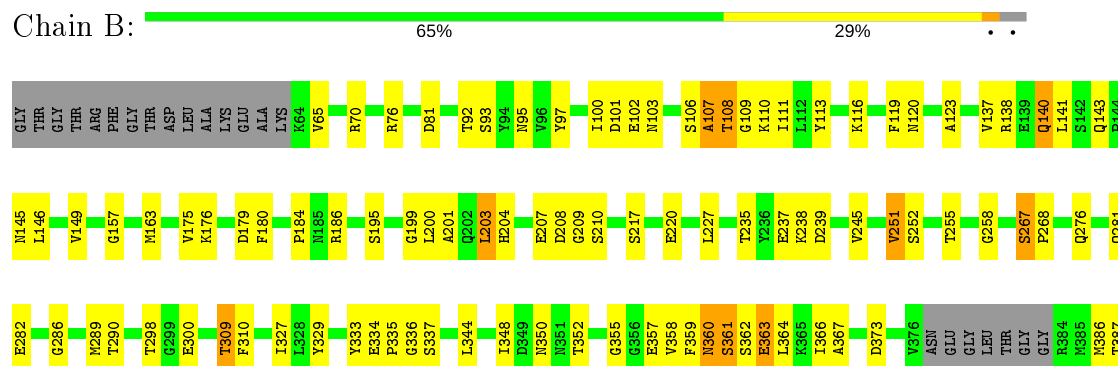
### 3 Residue-property plots

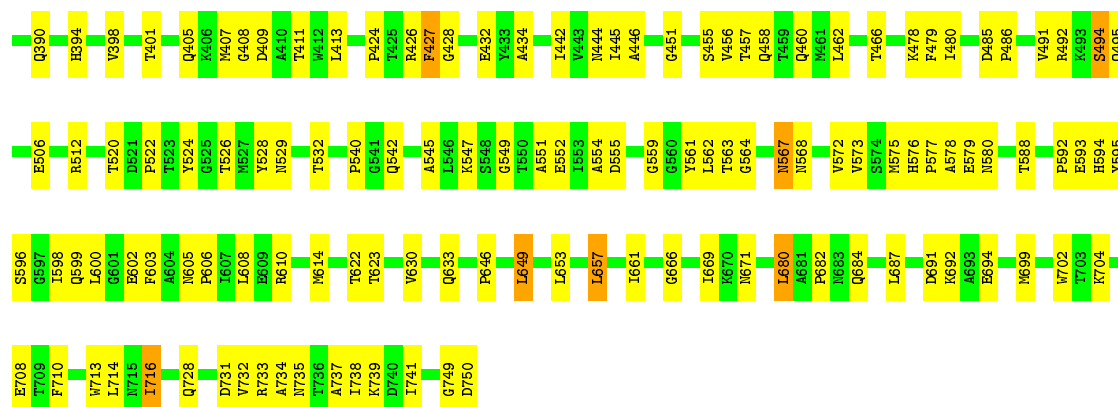
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: penicillin-binding protein 2x



- Molecule 1: penicillin-binding protein 2x





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.99Å 194.99Å 154.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.00 – 3.00 41.96 – 2.97	Depositor EDS
% Data completeness (in resolution range)	96.5 (42.00-3.00) 93.0 (41.96-2.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 2.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.231 , 0.256 0.215 , 0.244	Depositor DCC
$R_{free}$ test set	4725 reflections (8.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.8	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10315	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.38	0/5222	0.64	0/7101
1	B	0.38	0/5225	0.64	0/7098
All	All	0.38	0/10447	0.64	0/14199

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	5128	0	4890	186	0
1	B	5132	0	4917	172	1
2	A	5	0	0	2	0
2	B	5	0	0	0	0
3	A	19	0	0	0	0
3	B	26	0	0	1	0
All	All	10315	0	9807	358	1

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 18.

All (358) 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:710:PHE:CZ	1:B:714:LEU:HD12	1.84	1.11
1:A:111:ILE:H	1:A:111:ILE:HD12	1.17	1.09
1:B:596:SER:HB3	1:B:599:GLN:HE21	1.21	1.04
1:B:710:PHE:CZ	1:B:714:LEU:CD1	2.42	1.02
1:A:232:GLY:HA3	1:A:255:THR:HG22	1.47	0.95
1:A:615:LYS:HA	1:A:618:LEU:HD11	1.56	0.86
1:B:714:LEU:HD13	1:B:738:ILE:HD13	1.56	0.84
1:A:424:PRO:HG3	1:A:434:ALA:HB2	1.62	0.82
1:B:572:VAL:HG21	1:B:600:LEU:HD21	1.60	0.81
1:A:422:GLY:HA3	1:A:437:LEU:HD22	1.62	0.80
1:B:714:LEU:HD13	1:B:738:ILE:CD1	2.10	0.80
1:A:714:LEU:HD13	1:A:738:ILE:HD13	1.63	0.79
1:A:111:ILE:N	1:A:111:ILE:HD12	1.96	0.79
1:A:596:SER:HB3	1:A:599:GLN:HE21	1.47	0.79
1:B:111:ILE:HG23	1:B:113:TYR:CE1	2.18	0.78
1:A:188:TYR:O	1:A:313:ASP:HB2	1.84	0.78
1:B:710:PHE:CE1	1:B:714:LEU:HD11	2.18	0.78
1:A:286:GLY:HA2	1:A:592:PRO:HA	1.67	0.77
1:B:352:THR:O	1:B:352:THR:HG22	1.84	0.77
1:A:710:PHE:CZ	1:A:714:LEU:HD12	2.20	0.77
1:A:732:VAL:HG11	1:A:741:ILE:HD13	1.66	0.77
1:A:694:GLU:O	1:A:738:ILE:HG22	1.86	0.76
1:B:596:SER:HB3	1:B:599:GLN:NE2	1.98	0.76
1:A:143:GLN:HE21	1:A:149:VAL:HG21	1.51	0.75
1:B:309:THR:HG22	1:B:310:PHE:H	1.50	0.75
1:B:728:GLN:HG3	1:B:749:GLY:HA3	1.68	0.74
1:A:457:THR:OG1	1:A:460:GLN:HG3	1.86	0.74
1:B:572:VAL:HG21	1:B:600:LEU:CD2	2.17	0.73
1:A:736:THR:CG2	1:A:741:ILE:HD11	2.19	0.73
1:A:620:LEU:H	1:A:620:LEU:HD22	1.53	0.72
1:B:76:ARG:HD3	1:B:186:ARG:NE	2.05	0.72
1:B:424:PRO:HG3	1:B:434:ALA:HB2	1.72	0.72
1:A:239:ASP:OD2	1:A:243:ASN:HB2	1.90	0.72
1:A:227:LEU:O	1:A:258:GLY:HA3	1.89	0.71
1:B:298:THR:OG1	1:B:300:GLU:HG3	1.90	0.70
1:A:92:THR:HG23	1:A:184:PRO:HA	1.73	0.70
1:B:120:ASN:ND2	1:B:138:ARG:HD3	2.05	0.70
1:A:462:LEU:O	1:A:466:THR:HG23	1.91	0.70
1:B:710:PHE:CZ	1:B:714:LEU:HD11	2.22	0.70
1:A:549:GLY:HA2	2:A:751:SO4:O1	1.92	0.70
1:B:710:PHE:CE2	1:B:714:LEU:HD12	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:VAL:HG11	1:A:741:ILE:CD1	2.21	0.69
1:B:201:ALA:N	1:B:220:GLU:HG2	2.06	0.69
1:A:111:ILE:H	1:A:111:ILE:CD1	1.96	0.69
1:B:710:PHE:CE1	1:B:714:LEU:CD1	2.74	0.69
1:A:412:TRP:HE1	1:A:448:SER:HB2	1.56	0.68
1:B:352:THR:O	1:B:352:THR:CG2	2.42	0.68
1:A:447:MET:HA	1:A:450:PHE:CE1	2.29	0.67
1:A:290:THR:HG21	1:A:458:GLN:OE1	1.94	0.67
1:A:143:GLN:NE2	1:A:149:VAL:CG2	2.58	0.67
1:A:736:THR:HG21	1:A:741:ILE:HD11	1.77	0.66
1:B:290:THR:HB	1:B:588:THR:OG1	1.96	0.66
1:A:623:THR:HG21	1:A:628:GLU:OE1	1.95	0.66
1:B:457:THR:OG1	1:B:460:GLN:HG3	1.95	0.66
1:B:116:LYS:HA	1:B:119:PHE:CD1	2.31	0.66
1:B:281:GLN:HA	1:B:289:MET:HE2	1.75	0.66
1:A:716:ILE:N	1:A:716:ILE:HD13	2.11	0.65
1:B:290:THR:HG21	1:B:458:GLN:OE1	1.97	0.65
1:A:290:THR:HG21	1:A:458:GLN:HE22	1.62	0.65
1:A:143:GLN:HE21	1:A:149:VAL:CG2	2.10	0.64
1:A:491:VAL:HG22	1:A:492:ARG:N	2.11	0.64
1:A:563:THR:HG22	1:A:564:GLY:N	2.14	0.63
1:A:163:MET:HG3	1:A:180:PHE:CD2	2.34	0.63
1:A:407:MET:HG2	1:A:411:THR:HB	1.81	0.62
1:B:336:GLY:O	1:B:451:GLY:HA3	1.99	0.62
1:B:622:THR:OG1	1:B:623:THR:N	2.29	0.62
1:A:649:LEU:HD12	1:A:688:ILE:HD13	1.82	0.62
1:B:694:GLU:O	1:B:738:ILE:HG22	2.00	0.61
1:A:618:LEU:HD13	1:A:620:LEU:HD21	1.83	0.61
1:B:227:LEU:O	1:B:258:GLY:HA3	2.01	0.61
1:A:284:VAL:HG12	1:A:594:HIS:O	2.01	0.61
1:A:492:ARG:HG2	1:A:682:PRO:HG3	1.83	0.61
1:B:140:GLN:O	1:B:149:VAL:HG21	1.99	0.61
1:B:428:GLY:HA3	1:B:479:PHE:HE2	1.66	0.61
1:B:492:ARG:HG2	1:B:682:PRO:HG3	1.81	0.60
1:A:395:SER:O	1:A:395:SER:OG	2.17	0.60
1:B:562:LEU:HD13	1:B:567:ASN:HD21	1.66	0.60
1:A:558:ASN:N	1:A:558:ASN:HD22	2.00	0.60
1:A:414:ASP:O	1:A:418:ARG:HG3	2.02	0.60
1:B:123:ALA:HA	1:B:137:VAL:HG11	1.83	0.59
1:B:716:ILE:HD13	1:B:716:ILE:O	2.02	0.59
1:B:337:SER:HB2	1:B:549:GLY:HA2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:THR:HG21	1:A:458:GLN:NE2	2.17	0.59
1:B:478:LYS:HE2	1:B:495:GLN:O	2.02	0.59
1:B:143:GLN:NE2	1:B:149:VAL:HG23	2.17	0.59
1:A:563:THR:HG22	1:A:564:GLY:H	1.66	0.59
1:B:335:PRO:HD3	1:B:456:VAL:HG22	1.85	0.59
1:B:462:LEU:O	1:B:466:THR:HG23	2.02	0.59
1:B:491:VAL:HG22	1:B:492:ARG:N	2.17	0.59
1:A:140:GLN:O	1:A:143:GLN:HG3	2.02	0.59
1:A:443:VAL:O	1:A:447:MET:HG3	2.02	0.59
1:A:207:GLU:HG2	1:A:208:ASP:H	1.67	0.58
1:A:704:LYS:O	1:A:708:GLU:HG3	2.03	0.58
1:A:521:ASP:OD2	1:A:524:TYR:HB2	2.03	0.58
1:A:143:GLN:NE2	1:A:149:VAL:HG23	2.19	0.58
1:B:633:GLN:NE2	1:B:682:PRO:HD2	2.18	0.58
1:A:336:GLY:O	1:A:451:GLY:HA3	2.05	0.57
1:A:350:ASN:HD22	1:A:352:THR:CG2	2.17	0.57
1:B:413:LEU:HD11	1:B:445:ILE:HD13	1.86	0.57
1:B:699:MET:HG2	1:B:702:TRP:CZ3	2.40	0.57
1:A:280:PHE:O	1:A:284:VAL:HG22	2.05	0.57
1:A:466:THR:O	1:A:470:ASN:HB2	2.05	0.57
1:A:615:LYS:O	1:A:618:LEU:HD12	2.05	0.57
1:A:133:GLU:O	1:A:136:TYR:HB3	2.05	0.56
1:A:736:THR:HG22	1:A:741:ILE:HD11	1.86	0.56
1:B:140:GLN:CA	1:B:140:GLN:HE21	2.17	0.56
1:B:579:GLU:CD	1:B:579:GLU:H	2.08	0.56
1:A:649:LEU:HD12	1:A:688:ILE:CD1	2.35	0.56
1:B:111:ILE:HG23	1:B:113:TYR:CD1	2.41	0.56
1:B:329:TYR:HB2	1:B:432:GLU:HG3	1.88	0.56
1:B:657:LEU:HD23	1:B:657:LEU:N	2.21	0.56
1:A:522:PRO:HA	1:A:528:TYR:CD2	2.40	0.56
1:A:352:THR:HG23	1:A:352:THR:O	2.05	0.56
1:B:649:LEU:HD22	1:B:653:LEU:HG	1.88	0.56
1:B:563:THR:HG22	1:B:564:GLY:H	1.71	0.55
1:B:562:LEU:HD13	1:B:567:ASN:ND2	2.22	0.55
1:B:119:PHE:CE2	1:B:141:LEU:HB3	2.42	0.55
1:B:598:ILE:O	1:B:602:GLU:HG3	2.06	0.55
1:A:621:GLN:O	1:A:622:THR:HG23	2.06	0.55
1:B:506:GLU:N	1:B:506:GLU:OE1	2.29	0.55
1:B:562:LEU:CB	1:B:567:ASN:HD22	2.20	0.55
1:A:65:VAL:HG12	1:A:239:ASP:HA	1.88	0.55
1:B:235:THR:OG1	1:B:252:SER:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:GLN:NE2	1:B:524:TYR:CE2	2.75	0.55
1:A:618:LEU:CD1	1:A:620:LEU:HD21	2.37	0.54
1:B:106:SER:OG	1:B:110:LYS:HB2	2.07	0.54
1:B:480:ILE:HG21	1:B:657:LEU:HD21	1.88	0.54
1:A:439:ALA:HB3	1:A:444:ASN:OD1	2.08	0.54
1:A:670:LYS:O	1:A:671:ASN:HB2	2.08	0.54
1:B:362:SER:O	1:B:363:GLU:O	2.26	0.54
1:B:728:GLN:CG	1:B:749:GLY:HA3	2.37	0.54
1:A:394:HIS:O	1:A:395:SER:HB3	2.07	0.54
1:B:108:THR:O	1:B:108:THR:HG22	2.07	0.54
1:B:512:ARG:HD2	1:B:578:ALA:O	2.08	0.54
1:A:163:MET:HG3	1:A:180:PHE:CE2	2.42	0.54
1:A:558:ASN:N	1:A:558:ASN:ND2	2.56	0.54
1:A:512:ARG:O	1:A:516:VAL:HG23	2.08	0.53
1:B:97:TYR:CZ	1:B:179:ASP:HB2	2.43	0.53
1:A:547:LYS:NZ	2:A:751:SO4:O2	2.42	0.53
1:B:361:SER:HB3	1:B:386:MET:CE	2.38	0.53
1:B:552:GLU:HA	1:B:568:ASN:HD22	1.73	0.53
1:B:428:GLY:HA3	1:B:479:PHE:CE2	2.44	0.53
1:A:104:TYR:CE1	1:A:246:PRO:HG3	2.44	0.53
1:A:447:MET:HA	1:A:450:PHE:HE1	1.71	0.53
1:A:386:MET:HB3	1:A:390:GLN:HB2	1.90	0.53
1:B:373:ASP:OD1	1:B:398:VAL:HG23	2.09	0.53
1:A:551:ALA:HB3	1:A:569:ILE:HB	1.91	0.52
1:A:615:LYS:HA	1:A:618:LEU:CD1	2.34	0.52
1:A:495:GLN:HB2	1:A:683:ASN:ND2	2.25	0.52
1:B:704:LYS:O	1:B:708:GLU:HG3	2.10	0.52
1:B:593:GLU:HB3	1:B:594:HIS:CE1	2.44	0.52
1:A:731:ASP:OD1	1:A:745:LYS:N	2.32	0.51
1:A:290:THR:HB	1:A:588:THR:OG1	2.11	0.51
1:A:297:LYS:HA	1:A:470:ASN:HD21	1.76	0.51
1:A:596:SER:HB3	1:A:599:GLN:NE2	2.21	0.51
1:B:200:LEU:C	1:B:220:GLU:HG2	2.29	0.51
1:B:491:VAL:HG22	1:B:492:ARG:H	1.74	0.51
1:B:401:THR:O	1:B:405:GLN:HG2	2.09	0.51
1:B:480:ILE:CG2	1:B:657:LEU:HD21	2.39	0.51
1:B:610:ARG:HD2	1:B:614:MET:CE	2.40	0.51
1:A:130:LEU:HD12	1:A:132:MET:HE3	1.93	0.51
1:A:340:LYS:HD3	1:A:400:MET:HG3	1.92	0.51
1:A:734:ALA:O	1:A:735:ASN:HB2	2.11	0.51
1:A:208:ASP:O	1:A:210:SER:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:GLN:CA	1:B:140:GLN:NE2	2.74	0.51
1:B:336:GLY:HA3	1:B:551:ALA:HB2	1.94	0.50
1:B:101:ASP:OD1	1:B:103:ASN:HB2	2.12	0.50
1:B:184:PRO:O	1:B:203:LEU:HD11	2.11	0.50
1:A:371:ILE:CD1	1:A:401:THR:HG21	2.42	0.50
1:B:290:THR:HG21	1:B:458:GLN:HE22	1.77	0.50
1:B:555:ASP:HB3	1:B:559:GLY:O	2.11	0.50
1:A:208:ASP:C	1:A:210:SER:H	2.14	0.50
1:B:522:PRO:HA	1:B:528:TYR:CD2	2.46	0.50
1:B:749:GLY:O	1:B:750:ASP:HB2	2.12	0.50
1:B:238:LYS:HA	1:B:245:VAL:HG23	1.94	0.50
1:B:309:THR:CG2	1:B:310:PHE:H	2.16	0.50
1:B:95:ASN:O	1:B:180:PHE:HA	2.12	0.50
1:A:264:THR:HG21	1:A:300:GLU:HB3	1.94	0.50
1:B:120:ASN:HD22	1:B:138:ARG:HD3	1.77	0.50
1:B:143:GLN:NE2	1:B:149:VAL:CG2	2.75	0.50
1:B:554:ALA:HA	1:B:561:TYR:HD1	1.77	0.50
1:B:649:LEU:CD2	1:B:653:LEU:HG	2.42	0.50
1:A:195:SER:HB3	1:A:310:PHE:CE1	2.47	0.49
1:B:352:THR:HG21	1:B:407:MET:HB2	1.94	0.49
1:B:286:GLY:HA2	1:B:592:PRO:HA	1.93	0.49
1:A:290:THR:HG21	1:A:458:GLN:CD	2.33	0.49
1:A:335:PRO:HD3	1:A:456:VAL:HG22	1.94	0.49
1:B:93:SER:HB2	1:B:157:GLY:HA2	1.94	0.49
1:A:440:ASP:O	1:A:441:ASN:HB3	2.13	0.49
1:B:92:THR:OG1	1:B:184:PRO:HA	2.13	0.49
1:A:140:GLN:O	1:A:149:VAL:HG21	2.12	0.49
1:A:491:VAL:CG2	1:A:492:ARG:N	2.76	0.49
1:B:680:LEU:HD12	1:B:684:GLN:HE22	1.78	0.49
1:A:696:VAL:HG21	1:A:741:ILE:HD12	1.93	0.48
1:A:92:THR:HG23	1:A:184:PRO:CA	2.43	0.48
1:A:630:VAL:HG23	1:A:630:VAL:O	2.14	0.48
1:A:738:ILE:O	1:A:739:LYS:C	2.51	0.48
1:B:65:VAL:HG12	1:B:239:ASP:HA	1.95	0.48
1:A:163:MET:HG3	1:A:180:PHE:CG	2.48	0.48
1:A:264:THR:CG2	1:A:300:GLU:HB3	2.43	0.48
1:B:394:HIS:HA	1:B:526:THR:HG23	1.96	0.48
1:B:100:ILE:HD11	1:B:146:LEU:O	2.14	0.48
1:B:529:ASN:HB3	1:B:532:THR:HB	1.95	0.48
1:A:387:THR:O	1:A:388:PHE:C	2.51	0.48
1:A:579:GLU:CD	1:A:579:GLU:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:VAL:HG23	1:A:736:THR:O	2.14	0.48
1:A:337:SER:HB2	1:A:549:GLY:CA	2.44	0.48
1:B:116:LYS:HA	1:B:119:PHE:CE1	2.49	0.48
1:B:106:SER:O	1:B:107:ALA:C	2.52	0.47
1:B:140:GLN:HA	1:B:140:GLN:NE2	2.28	0.47
1:B:333:TYR:O	1:B:455:SER:HA	2.13	0.47
1:B:309:THR:HG22	1:B:310:PHE:N	2.26	0.47
1:B:344:LEU:O	1:B:348:ILE:HG13	2.14	0.47
1:A:472:GLY:O	1:A:502:PRO:HD2	2.14	0.47
1:B:592:PRO:HG3	1:B:595:TYR:HB2	1.95	0.47
1:B:163:MET:HG3	1:B:180:PHE:CD2	2.49	0.47
1:B:731:ASP:OD1	1:B:732:VAL:N	2.40	0.47
1:A:207:GLU:HG2	1:A:208:ASP:N	2.30	0.47
1:A:413:LEU:HD23	1:A:416:LEU:HD12	1.95	0.47
1:A:621:GLN:O	1:A:622:THR:CG2	2.63	0.47
1:B:276:GLN:HB3	1:B:603:PHE:CD1	2.50	0.47
1:A:104:TYR:CD1	1:A:246:PRO:HG3	2.49	0.47
1:A:91:ALA:O	1:A:185:ASN:HB3	2.15	0.47
1:A:618:LEU:HD13	1:A:620:LEU:CD2	2.45	0.47
1:A:279:ALA:O	1:A:282:GLU:HB3	2.15	0.46
1:B:366:ILE:O	1:B:367:ALA:HB3	2.14	0.46
1:A:298:THR:OG1	1:A:300:GLU:HG3	2.15	0.46
1:A:424:PRO:HG3	1:A:434:ALA:CB	2.42	0.46
1:B:494:SER:CB	1:B:657:LEU:HD13	2.45	0.46
1:B:680:LEU:HD12	1:B:684:GLN:NE2	2.31	0.46
1:A:714:LEU:O	1:A:715:ASN:CB	2.63	0.46
1:A:736:THR:O	1:A:737:ALA:C	2.54	0.46
1:B:251:VAL:O	1:B:251:VAL:CG2	2.63	0.46
1:A:297:LYS:HE2	1:A:580:ASN:HD21	1.80	0.46
1:A:666:GLY:HA3	1:A:691:ASP:OD1	2.15	0.46
1:B:576:HIS:HA	1:B:577:PRO:C	2.36	0.46
1:A:350:ASN:ND2	1:A:352:THR:HB	2.30	0.46
1:A:622:THR:HB	1:A:623:THR:H	1.55	0.46
1:A:598:ILE:O	1:A:602:GLU:HG3	2.16	0.46
1:A:437:LEU:HD12	1:A:438:PRO:HD2	1.97	0.45
1:A:566:THR:O	1:A:591:GLN:HA	2.16	0.45
1:A:572:VAL:HG21	1:A:600:LEU:CD2	2.46	0.45
1:A:371:ILE:HD12	1:A:401:THR:HG21	1.98	0.45
1:B:290:THR:HG21	1:B:458:GLN:NE2	2.31	0.45
1:B:358:VAL:HG12	1:B:359:PHE:N	2.31	0.45
1:B:646:PRO:HG3	1:B:669:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:PHE:H	1:A:427:PHE:HD1	1.65	0.45
1:B:355:GLY:O	1:B:387:THR:HB	2.16	0.45
1:B:357:GLU:O	1:B:387:THR:HA	2.17	0.45
1:A:238:LYS:HA	1:A:243:ASN:O	2.16	0.45
1:B:65:VAL:HG21	1:B:237:GLU:OE1	2.17	0.45
1:A:272:PHE:O	1:A:275:THR:HB	2.17	0.45
1:A:297:LYS:CE	1:A:580:ASN:HD21	2.30	0.45
1:B:610:ARG:HD2	1:B:614:MET:HE3	1.99	0.45
1:A:398:VAL:O	1:A:402:LEU:HG	2.16	0.45
1:A:171:GLU:C	1:A:173:ALA:H	2.20	0.44
1:A:359:PHE:CZ	1:A:386:MET:HE3	2.53	0.44
1:B:195:SER:HB3	1:B:310:PHE:CE1	2.52	0.44
1:B:387:THR:OG1	1:B:390:GLN:HG3	2.17	0.44
1:A:350:ASN:HD22	1:A:352:THR:HB	1.83	0.44
1:A:116:LYS:HA	1:A:119:PHE:CD1	2.52	0.44
1:A:162:ASN:O	1:A:166:ILE:HG13	2.17	0.44
1:A:387:THR:O	1:A:389:SER:N	2.50	0.44
1:A:420:LYS:NZ	1:A:499:VAL:O	2.50	0.44
1:B:120:ASN:HD21	1:B:138:ARG:HD3	1.80	0.44
1:A:149:VAL:HG22	1:A:150:SER:N	2.32	0.44
1:B:282:GLU:HA	1:B:282:GLU:OE1	2.18	0.44
1:B:506:GLU:H	1:B:506:GLU:CD	2.18	0.44
1:A:362:SER:HA	1:A:383:GLY:HA3	1.99	0.44
1:A:394:HIS:HA	1:A:524:TYR:O	2.17	0.44
1:A:495:GLN:HB2	1:A:683:ASN:CG	2.37	0.44
1:A:199:GLY:HA3	1:A:217:SER:O	2.17	0.44
1:A:491:VAL:HG22	1:A:492:ARG:H	1.81	0.44
1:A:497:GLU:HG3	1:A:659:GLN:CD	2.38	0.44
1:A:699:MET:HG2	1:A:702:TRP:CZ3	2.52	0.44
1:B:267:SER:N	1:B:268:PRO:CD	2.81	0.44
1:B:106:SER:O	1:B:109:GLY:N	2.51	0.43
1:A:749:GLY:O	1:A:750:ASP:HB2	2.18	0.43
1:B:562:LEU:HB2	1:B:567:ASN:HD22	1.82	0.43
1:B:661:ILE:HB	1:B:687:LEU:HD23	2.00	0.43
1:A:605:ASN:HB2	1:A:606:PRO:HD3	2.00	0.43
1:A:628:GLU:HA	1:A:628:GLU:OE1	2.19	0.43
1:A:714:LEU:HD23	1:A:714:LEU:HA	1.86	0.43
1:B:572:VAL:HG21	1:B:600:LEU:HD22	1.99	0.43
1:B:576:HIS:CE1	1:B:608:LEU:HD22	2.53	0.43
1:A:140:GLN:OE1	1:A:140:GLN:HA	2.18	0.43
1:A:276:GLN:HB3	1:A:603:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:SER:HB3	1:B:386:MET:HE2	2.00	0.43
1:A:101:ASP:OD1	1:A:104:TYR:HB2	2.19	0.43
1:A:275:THR:HG22	1:A:276:GLN:N	2.33	0.43
1:A:337:SER:HB2	1:A:549:GLY:HA3	2.00	0.43
1:A:563:THR:CG2	1:A:564:GLY:N	2.82	0.43
1:B:716:ILE:C	1:B:716:ILE:HD13	2.39	0.43
1:A:116:LYS:HA	1:A:119:PHE:CE1	2.54	0.42
1:A:96:VAL:HB	1:A:180:PHE:CE2	2.54	0.42
1:A:358:VAL:HG12	1:A:359:PHE:N	2.34	0.42
1:B:426:ARG:HD2	3:B:21:HOH:O	2.19	0.42
1:A:185:ASN:HD22	1:A:185:ASN:HA	1.70	0.42
1:A:292:THR:HG23	1:A:304:THR:HB	2.01	0.42
1:A:359:PHE:HZ	1:A:386:MET:HE3	1.84	0.42
1:B:123:ALA:CB	1:B:137:VAL:HB	2.50	0.42
1:B:350:ASN:ND2	1:B:352:THR:OG1	2.53	0.42
1:B:671:ASN:ND2	1:B:713:TRP:CE2	2.87	0.42
1:B:102:GLU:HA	1:B:113:TYR:CE2	2.54	0.42
1:B:485:ASP:HA	1:B:486:PRO:HD2	1.93	0.42
1:A:593:GLU:HB3	1:A:594:HIS:CD2	2.54	0.42
1:A:714:LEU:HD13	1:A:738:ILE:CD1	2.42	0.42
1:A:491:VAL:O	1:A:633:GLN:HA	2.19	0.42
1:A:219:MET:O	1:A:220:GLU:C	2.58	0.42
1:A:542:GLN:NE2	1:A:577:PRO:HB3	2.34	0.42
1:B:251:VAL:O	1:B:251:VAL:HG22	2.19	0.42
1:B:737:ALA:O	1:B:741:ILE:HD13	2.20	0.42
1:A:428:GLY:HA3	1:A:479:PHE:CE2	2.54	0.42
1:B:180:PHE:CD1	1:B:180:PHE:N	2.88	0.42
1:B:732:VAL:HG11	1:B:741:ILE:HG12	2.02	0.42
1:B:334:GLU:HA	1:B:335:PRO:HD2	1.82	0.41
1:B:360:ASN:HD22	1:B:361:SER:N	2.18	0.41
1:B:408:GLY:O	1:B:409:ASP:C	2.58	0.41
1:B:199:GLY:HA3	1:B:217:SER:O	2.19	0.41
1:A:359:PHE:CZ	1:A:386:MET:CE	3.03	0.41
1:A:640:SER:HB2	1:A:676:GLU:OE2	2.20	0.41
1:A:463:ARG:O	1:A:474:MET:HG3	2.21	0.41
1:B:605:ASN:HB2	1:B:606:PRO:HD3	2.02	0.41
1:A:348:ILE:HG21	1:A:507:ALA:HA	2.03	0.41
1:A:374:TRP:CG	1:A:375:ASP:N	2.89	0.41
1:A:711:ALA:HA	1:A:716:ILE:HD11	2.02	0.41
1:B:327:ILE:HG13	1:B:327:ILE:H	1.72	0.41
1:A:424:PRO:CG	1:A:434:ALA:HB2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LEU:HA	1:A:437:LEU:HD13	1.91	0.41
1:B:208:ASP:C	1:B:210:SER:H	2.23	0.41
1:B:336:GLY:CA	1:B:551:ALA:HB2	2.51	0.41
1:B:407:MET:SD	1:B:411:THR:HG22	2.61	0.41
1:B:424:PRO:HG3	1:B:434:ALA:CB	2.47	0.41
1:B:547:LYS:HA	1:B:547:LYS:HD2	1.86	0.41
1:B:666:GLY:HA3	1:B:691:ASP:OD1	2.20	0.41
1:A:547:LYS:HD2	1:A:547:LYS:HA	1.92	0.41
1:B:175:VAL:HG12	1:B:176:LYS:N	2.35	0.41
1:B:699:MET:HG2	1:B:702:TRP:CE3	2.55	0.41
1:B:734:ALA:O	1:B:735:ASN:HB2	2.19	0.41
1:B:545:ALA:HB3	1:B:575:MET:HB2	2.02	0.41
1:B:610:ARG:HD2	1:B:614:MET:HE1	2.03	0.41
1:B:741:ILE:N	1:B:741:ILE:HD12	2.36	0.41
1:A:696:VAL:HA	1:A:697:PRO:HD3	1.82	0.41
1:A:357:GLU:OE1	1:A:406:LYS:HE3	2.21	0.40
1:A:357:GLU:O	1:A:387:THR:HA	2.21	0.40
1:A:572:VAL:HG21	1:A:600:LEU:HD21	2.03	0.40
1:A:102:GLU:HA	1:A:113:TYR:CZ	2.56	0.40
1:A:193:PHE:O	1:A:193:PHE:HD1	2.04	0.40
1:A:689:LEU:HB2	1:A:713:TRP:CZ3	2.57	0.40
1:B:694:GLU:C	1:B:738:ILE:HG22	2.41	0.40
1:B:427:PHE:H	1:B:427:PHE:HD1	1.68	0.40
1:B:522:PRO:HB3	1:B:528:TYR:CZ	2.56	0.40
1:B:563:THR:HG22	1:B:564:GLY:N	2.34	0.40
1:B:542:GLN:HA	1:B:542:GLN:NE2	2.36	0.40
1:B:573:VAL:O	1:B:573:VAL:HG13	2.21	0.40
1:A:140:GLN:HG2	1:A:150:SER:O	2.21	0.40
1:A:699:MET:HE1	1:A:746:LEU:HD11	2.02	0.40
1:B:444:ASN:C	1:B:446:ALA:N	2.75	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:HIS:CE1	1:B:207:GLU:OE2[6_566]	2.09	0.11

## 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	685/702 (98%)	622 (91%)	52 (8%)	11 (2%)	9	40
1	B	676/702 (96%)	616 (91%)	51 (8%)	9 (1%)	12	45
All	All	1361/1404 (97%)	1238 (91%)	103 (8%)	20 (2%)	10	42

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	698	ASP
1	B	363	GLU
1	A	630	VAL
1	A	739	LYS
1	A	208	ASP
1	A	388	PHE
1	A	578	ALA
1	A	692	LYS
1	A	715	ASN
1	B	108	THR
1	B	442	ILE
1	B	692	LYS
1	A	209	GLY
1	A	441	ASN
1	A	615	LYS
1	B	107	ALA
1	B	145	ASN
1	B	739	LYS
1	B	361	SER
1	B	209	GLY

### 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	538/591 (91%)	510 (95%)	28 (5%)	23	59
1	B	544/591 (92%)	522 (96%)	22 (4%)	31	68
All	All	1082/1182 (92%)	1032 (95%)	50 (5%)	27	64

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ASP
1	A	101	ASP
1	A	111	ILE
1	A	140	GLN
1	A	183	SER
1	A	185	ASN
1	A	207	GLU
1	A	255	THR
1	A	309	THR
1	A	338	THR
1	A	368	ASP
1	A	387	THR
1	A	427	PHE
1	A	437	LEU
1	A	495	GLN
1	A	501	ASN
1	A	520	THR
1	A	529	ASN
1	A	580	ASN
1	A	593	GLU
1	A	594	HIS
1	A	618	LEU
1	A	623	THR
1	A	695	GLU
1	A	716	ILE
1	A	728	GLN
1	A	733	ARG
1	A	750	ASP
1	B	70	ARG
1	B	81	ASP
1	B	140	GLN

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Mol	Chain	Res	Type
1	B	203	LEU
1	B	251	VAL
1	B	255	THR
1	B	267	SER
1	B	309	THR
1	B	360	ASN
1	B	364	LEU
1	B	427	PHE
1	B	494	SER
1	B	520	THR
1	B	540	PRO
1	B	567	ASN
1	B	580	ASN
1	B	630	VAL
1	B	649	LEU
1	B	657	LEU
1	B	680	LEU
1	B	716	ILE
1	B	733	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	185	ASN
1	A	243	ASN
1	A	350	ASN
1	A	377	ASN
1	A	470	ASN
1	A	495	GLN
1	A	501	ASN
1	A	529	ASN
1	A	542	GLN
1	A	558	ASN
1	A	568	ASN
1	A	580	ASN
1	A	599	GLN
1	A	659	GLN
1	B	120	ASN
1	B	140	GLN
1	B	143	GLN
1	B	202	GLN

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Mol	Chain	Res	Type
1	B	206	ASN
1	B	350	ASN
1	B	360	ASN
1	B	444	ASN
1	B	501	ASN
1	B	514	HIS
1	B	542	GLN
1	B	567	ASN
1	B	568	ASN
1	B	580	ASN
1	B	599	GLN
1	B	633	GLN
1	B	684	GLN

### 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](#)

2 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	751	-	4,4,4	0.39	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	751	-	4,4,4	0.37	0	6,6,6	0.21	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	751	SO4	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	687/702 (97%)	-0.47	1 (0%) 95 89	36, 59, 91, 100	0
1	B	680/702 (96%)	-0.60	0 100 100	27, 52, 88, 100	0
All	All	1367/1404 (97%)	-0.53	1 (0%) 95 89	27, 55, 90, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	558	ASN	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	A	751	5/5	0.68	0.45	58,59,59,59	5
2	SO4	B	751	5/5	0.82	0.33	53,53,54,55	5



## 6.5 Other polymers [i](#)

There are no such residues in this entry.