Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 11:36 AM EDT

PDB ID	:	2Y59
Title	:	Unexpected tricovalent binding mode of boronic acids within the active site of a penicillin binding protein
Authors	:	Sauvage, E.; Zervosen, A.; Herman, R.; Kerff, F.; Rocaboy, M.; Charlier, P.
Deposited on	:	2011-01-12
Resolution	:	2.50 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:

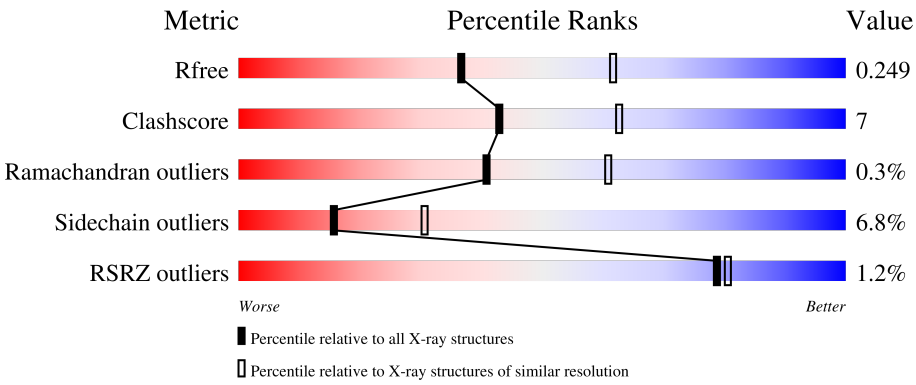
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	466	% 80% 17% •
1	B	466	% 86% 11% •
1	C	466	% 88% 10% •
1	D	466	2% 82% 17% •

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
3	SO4	D	501	-	-	X	-

2 Entry composition (i)

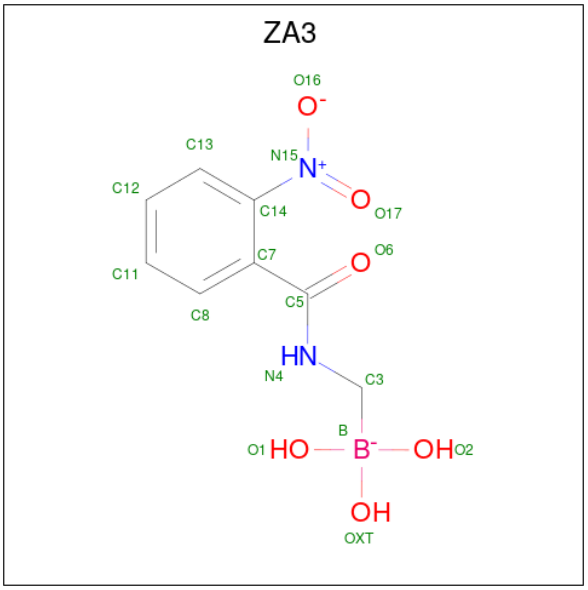
There are 5 unique types of molecules in this entry. The entry contains 13987 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-ALANYL-D-ALANINE CARBOXYPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	466	3353	2076	564	707	6	0	0	0
1	B	466	3344	2071	564	703	6	0	0	1
1	C	466	3344	2071	564	703	6	0	0	1
1	D	466	3353	2076	564	707	6	0	0	0

- Molecule 2 is TRIHYDROXY-[[(2-NITROPHENYL)CARBONYLAMINO]METHYL]BORON (three-letter code: ZA3) (formula: $C_8H_{10}BN_2O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	B	C	N	O		
2	A	1	16	1	8	2	5	0	0
2	B	1	14	1	8	2	3	0	0

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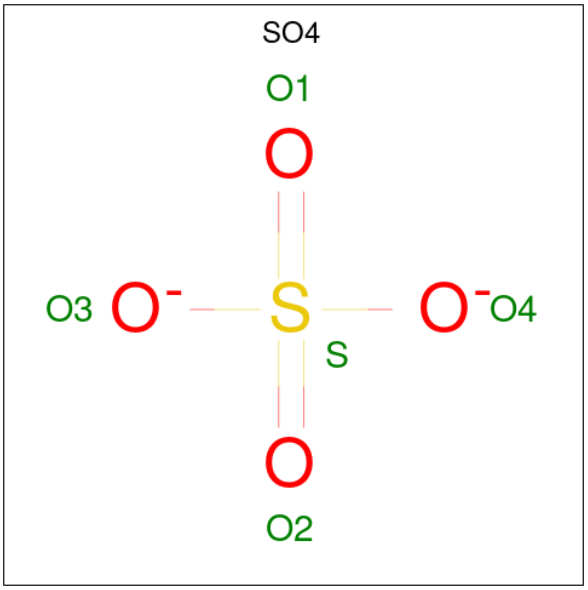
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	B	C	N	O		
2	C	1	14	1	8	2	3	0	0
			Total	B	C	N	O		
2	D	1	16	1	8	2	5	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	104	Total O 104 104	0	0
5	B	113	Total O 113 113	0	0
5	C	127	Total O 127 127	0	0

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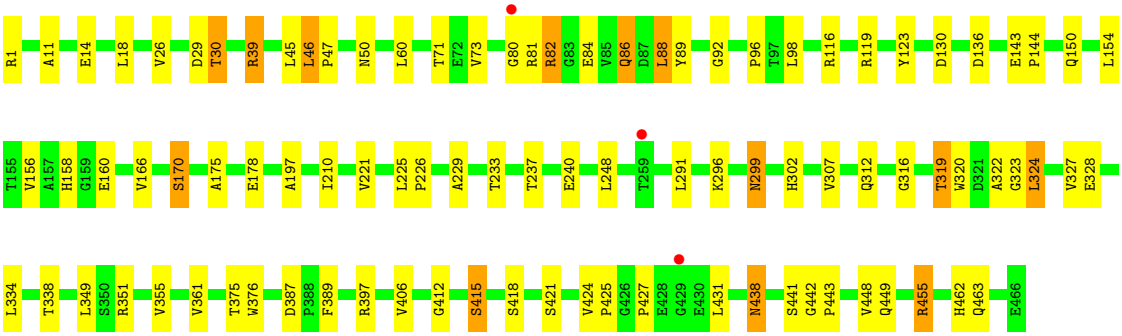
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	D	80	80	80	0	0

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.

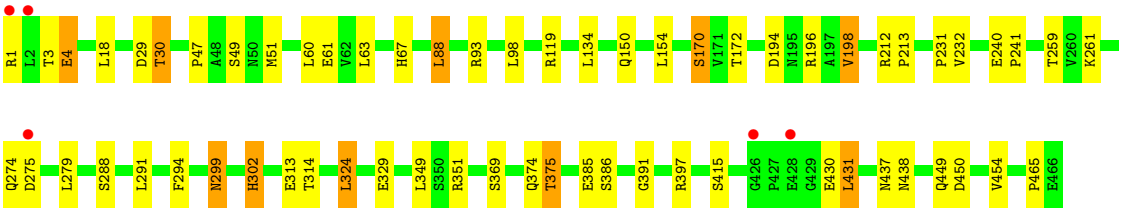
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain A:



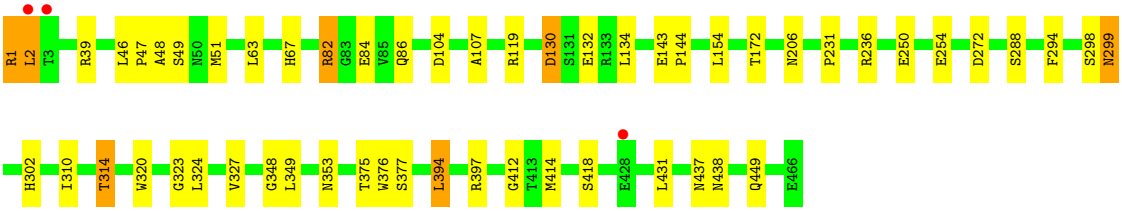
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain B:



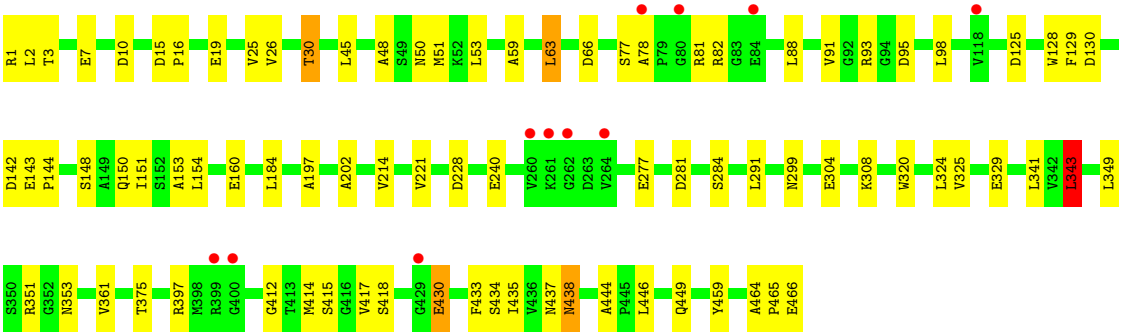
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain C:



• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain D:


R1 L2 T3 E7 D10 D15 P16 E19 V25 V26 T30 L45 A48 S49 N50 M51 K52 L53 A59 L63 D66 S77 A78 P79 G80 R81 R82 G83 E84 L88 V91 G92 R93 G94 D95 L98 V118 D125 W128 F129 D130
D142 E143 P144 S148 A149 Q150 I151 S152 A153 L154 E160 L184 A197 A202 V214 V221 D228 E240 V260 K261 G262 D263 V264 E277 D281 S284 L291 N299 E304 K308 W320 L324 V325 E329 L341 V342 L343 L349
S350 R351 G352 N353 V361 T375 R397 M398 R399 G400 G412 T413 M414 S415 G416 V417 S418 G429 E430 F433 S434 I435 V436 M437 M438 A444 P445 L446 Q449 Y459 A464 P465 E466

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.88Å 91.35Å 106.92Å 90.00° 94.27° 90.00°	Depositor
Resolution (Å)	42.00 – 2.50 41.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.00-2.50) 99.8 (41.99-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.195 , 0.254 0.192 , 0.249	Depositor DCC
R_{free} test set	3493 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13987	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZA3, 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	0.64	0/3412	0.72	1/4666 (0.0%)
1	B	0.61	0/3403	0.72	2/4656 (0.0%)
1	C	0.63	0/3403	0.72	0/4656
1	D	0.58	0/3412	0.71	2/4666 (0.0%)
All	All	0.62	0/13630	0.71	5/18644 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	343	LEU	CA-CB-CG	6.43	130.09	115.30
1	A	46	LEU	CA-CB-CG	5.48	127.91	115.30
1	D	341	LEU	CA-CB-CG	5.45	127.84	115.30
1	B	198	VAL	CB-CA-C	-5.28	101.38	111.40
1	B	324	LEU	CB-CG-CD1	5.07	119.61	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	3353	0	3200	63	0
1	B	3344	0	3193	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3344	0	3193	31	0
1	D	3353	0	3200	40	0
2	A	16	0	9	3	0
2	B	14	0	7	3	0
2	C	14	0	7	3	0
2	D	16	0	9	2	0
3	A	25	0	0	1	0
3	B	25	0	0	0	0
3	C	25	0	0	1	0
3	D	30	0	0	3	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	A	104	0	0	2	0
5	B	113	0	0	1	0
5	C	127	0	0	1	0
5	D	80	0	0	3	0
All	All	13987	0	12818	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 7.

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)
3:D:501:SO4:S	5:D:2001:HOH:O	2.10	1.07
1:A:86:GLN:HE22	1:A:119:ARG:HD2	1.27	0.97
1:A:319:THR:HG22	1:A:322:ALA:H	1.31	0.92
1:B:299:ASN:ND2	1:B:302:HIS:H	1.71	0.86
1:B:288:SER:HB2	1:B:375:THR:HG21	1.59	0.85
3:D:501:SO4:O1	5:D:2001:HOH:O	1.93	0.79
1:A:406:VAL:HG13	1:A:425:PRO:HD2	1.63	0.78
1:C:397:ARG:HH22	1:C:449:GLN:HE21	1.31	0.76
1:C:1:ARG:HG2	1:C:2:LEU:H	1.51	0.76
1:D:202:ALA:HB1	1:D:228:ASP:OD2	1.85	0.76
1:B:63:LEU:O	1:B:67:HIS:HB2	1.87	0.74
1:B:172:THR:HG22	1:B:231:PRO:HB3	1.68	0.73
1:B:1:ARG:HG2	1:B:4:GLU:HB2	1.71	0.72
1:C:47:PRO:HG3	1:C:51:MET:HE2	1.71	0.71
1:A:1:ARG:HH22	1:A:455:ARG:NH2	1.88	0.71
3:D:501:SO4:O2	5:D:2001:HOH:O	2.02	0.69
1:B:47:PRO:HG3	1:B:51:MET:HE2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:GLY:O	1:D:418:SER:HA	1.91	0.69
1:C:49:SER:HB2	2:C:501:ZA3:O17	1.92	0.68
1:A:412:GLY:HA2	2:A:501:ZA3:O2	1.94	0.68
1:B:49:SER:HB2	2:B:501:ZA3:O17	1.96	0.66
2:C:501:ZA3:O17	2:C:501:ZA3:C5	2.44	0.66
1:A:86:GLN:NE2	1:A:119:ARG:HD2	2.07	0.66
1:A:387:ASP:OD1	5:A:601:HOH:O	2.14	0.64
1:A:406:VAL:HG21	1:A:462:HIS:CE1	2.32	0.64
1:C:47:PRO:HG3	1:C:51:MET:CE	2.28	0.64
1:A:81:ARG:HD3	1:B:313:GLU:OE2	1.98	0.63
1:B:47:PRO:HG3	1:B:51:MET:CE	2.28	0.63
1:A:312:GLN:NE2	1:A:316:GLY:HA2	2.13	0.63
1:C:172:THR:HG22	1:C:231:PRO:HB3	1.79	0.63
1:D:78:ALA:HA	1:D:277:GLU:HG2	1.80	0.62
1:B:299:ASN:HD22	1:B:299:ASN:C	2.02	0.62
1:A:26:VAL:HG12	1:A:361:VAL:HG21	1.82	0.61
2:B:501:ZA3:O17	2:B:501:ZA3:C5	2.49	0.61
1:A:319:THR:CG2	1:A:322:ALA:H	2.09	0.61
1:B:397:ARG:HH22	1:B:449:GLN:HE21	1.48	0.61
1:C:1:ARG:CG	1:C:2:LEU:H	2.13	0.61
1:B:119:ARG:HG2	1:B:119:ARG:HH11	1.67	0.60
1:B:294:PHE:HB2	1:B:302:HIS:HD2	1.68	0.59
1:D:397:ARG:HH22	1:D:449:GLN:HE21	1.50	0.58
1:A:412:GLY:O	1:A:418:SER:HA	2.04	0.58
1:D:7:GLU:HA	1:D:10:ASP:HB2	1.85	0.58
1:C:323:GLY:O	1:C:327:VAL:HG23	2.03	0.58
1:D:197:ALA:HB2	1:D:221:VAL:HG12	1.86	0.57
1:A:1:ARG:HH22	1:A:455:ARG:HH22	1.52	0.57
1:A:158:HIS:HD2	5:A:640:HOH:O	1.87	0.56
1:B:351:ARG:NH2	1:B:415:SER:O	2.38	0.56
1:D:1:ARG:HH21	1:D:459:TYR:HA	1.71	0.56
1:A:150:GLN:HE22	1:A:240:GLU:H	1.53	0.56
1:C:236:ARG:NH1	3:C:503:SO4:O2	2.33	0.56
1:B:150:GLN:NE2	1:B:240:GLU:H	2.04	0.56
1:C:397:ARG:NH2	1:C:449:GLN:HE21	2.03	0.56
1:A:160:GLU:HG2	3:A:506:SO4:O2	2.06	0.55
1:A:60:LEU:HD11	1:A:291:LEU:HD11	1.87	0.55
1:A:299:ASN:ND2	1:A:302:HIS:H	2.04	0.55
1:D:93:ARG:HG2	1:D:128:TRP:CG	2.41	0.55
1:A:84:GLU:OE1	1:A:119:ARG:NH2	2.40	0.55
1:B:29:ASP:HA	1:B:431:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:HD12	1:A:226:PRO:HD2	1.88	0.55
1:A:73:VAL:HG12	1:A:88:LEU:CD2	2.37	0.54
1:B:170:SER:HA	1:B:232:VAL:O	2.07	0.53
1:C:82:ARG:HB3	1:C:84:GLU:HG3	1.90	0.53
1:A:307:VAL:HG11	1:A:324:LEU:HD13	1.91	0.53
1:C:397:ARG:HH22	1:C:449:GLN:NE2	2.03	0.53
1:A:1:ARG:HH12	1:A:455:ARG:HH22	1.56	0.53
1:A:397:ARG:HH22	1:A:449:GLN:HE21	1.56	0.52
1:A:1:ARG:NH2	1:A:455:ARG:HH22	2.07	0.52
1:D:93:ARG:HG2	1:D:128:TRP:CD2	2.45	0.52
1:A:50:ASN:ND2	1:A:421:SER:OG	2.42	0.52
1:D:412:GLY:HA2	2:D:502:ZA3:O2	2.09	0.52
1:C:310:ILE:O	1:C:314:THR:HB	2.09	0.52
1:A:73:VAL:HG12	1:A:88:LEU:HD21	1.93	0.51
1:C:1:ARG:HG2	1:C:2:LEU:N	2.24	0.51
1:C:130:ASP:HB3	1:C:132:GLU:H	1.76	0.51
1:D:48:ALA:HB1	2:D:502:ZA3:H32C	1.93	0.51
1:D:59:ALA:O	1:D:63:LEU:HB2	2.11	0.51
1:B:150:GLN:HE22	1:B:240:GLU:H	1.60	0.50
1:B:299:ASN:ND2	1:B:299:ASN:C	2.64	0.50
1:A:80:GLY:HA2	1:B:314:THR:O	2.12	0.50
1:B:93:ARG:NH1	5:B:604:HOH:O	2.44	0.50
1:A:197:ALA:HB2	1:A:221:VAL:HG12	1.94	0.49
1:B:119:ARG:HG2	1:B:119:ARG:NH1	2.27	0.49
1:B:60:LEU:HD11	1:B:291:LEU:HD11	1.94	0.49
1:A:351:ARG:NH2	1:A:415:SER:O	2.43	0.49
1:A:296:LYS:HE3	1:A:389:PHE:O	2.13	0.48
1:A:84:GLU:CD	1:A:119:ARG:NH2	2.67	0.48
1:A:299:ASN:HD22	1:A:302:HIS:H	1.60	0.48
1:C:48:ALA:O	1:C:348:GLY:HA3	2.13	0.48
1:C:51:MET:HE3	1:C:353:ASN:HB3	1.95	0.48
1:B:49:SER:CB	2:B:501:ZA3:C3	2.90	0.48
1:B:437:ASN:C	1:B:438:ASN:HD22	2.17	0.48
1:A:424:VAL:HB	1:A:431:LEU:HB2	1.97	0.47
1:C:412:GLY:O	1:C:418:SER:HA	2.14	0.47
1:A:1:ARG:NH1	1:A:455:ARG:HH22	2.10	0.47
1:D:325:VAL:O	1:D:329:GLU:HG3	2.14	0.47
1:A:84:GLU:CD	1:A:119:ARG:HH22	2.17	0.47
1:A:156:VAL:HG21	1:A:248:LEU:HD12	1.95	0.47
1:D:130:ASP:OD1	1:D:130:ASP:C	2.53	0.47
1:C:394:LEU:HD12	1:C:397:ARG:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:LEU:HD12	1:C:394:LEU:HA	1.84	0.47
1:D:30:THR:HB	1:D:430:GLU:O	2.15	0.47
1:D:151:ILE:HD12	1:D:304:GLU:HB2	1.97	0.46
1:B:397:ARG:NH2	1:B:449:GLN:HE21	2.13	0.46
1:C:298:SER:CB	2:C:501:ZA3:C3	2.93	0.46
1:D:150:GLN:NE2	1:D:240:GLU:H	2.14	0.46
1:D:414:MET:HB3	1:D:417:VAL:HB	1.98	0.46
1:C:143:GLU:N	1:C:144:PRO:CD	2.79	0.46
1:D:91:VAL:HA	1:D:125:ASP:HB3	1.97	0.46
1:A:166:VAL:HG12	1:A:237:THR:HA	1.98	0.46
1:A:175:ALA:HB3	1:A:178:GLU:OE1	2.17	0.45
1:D:51:MET:HE2	1:D:353:ASN:HB3	1.98	0.45
1:D:444:ALA:O	1:D:446:LEU:HG	2.16	0.45
1:A:143:GLU:N	1:A:144:PRO:CD	2.79	0.45
1:C:104:ASP:O	1:C:107:ALA:HB3	2.15	0.45
1:D:26:VAL:HG12	1:D:361:VAL:HG21	1.98	0.45
1:D:129:PHE:CG	1:D:153:ALA:HB2	2.51	0.45
1:A:71:THR:HG23	1:A:92:GLY:HA2	1.98	0.45
1:A:397:ARG:HH22	1:A:449:GLN:NE2	2.14	0.44
1:B:450:ASP:O	1:B:454:VAL:HG23	2.17	0.44
1:C:288:SER:HB2	1:C:375:THR:OG1	2.18	0.44
1:B:212:ARG:O	1:B:213:PRO:C	2.56	0.44
1:A:130:ASP:OD1	1:A:130:ASP:C	2.56	0.44
2:A:501:ZA3:N4	2:A:501:ZA3:O1	2.50	0.44
1:D:45:LEU:HD22	1:D:438:ASN:HB2	2.00	0.43
1:A:89:TYR:CE1	1:A:123:TYR:HB2	2.53	0.43
1:A:328:GLU:OE2	1:A:338:THR:OG1	2.25	0.43
1:B:299:ASN:HD21	1:B:302:HIS:H	1.57	0.43
1:A:39:ARG:HE	1:A:39:ARG:HB2	1.59	0.43
1:B:88:LEU:HD21	1:B:279:LEU:HD12	2.00	0.43
1:D:343:LEU:HD23	1:D:343:LEU:N	2.33	0.43
1:A:47:PRO:HG3	1:A:355:VAL:HG13	1.99	0.43
1:C:51:MET:CE	1:C:353:ASN:HB3	2.49	0.43
1:D:150:GLN:HE22	1:D:240:GLU:H	1.67	0.43
1:D:397:ARG:HH22	1:D:449:GLN:NE2	2.15	0.43
1:C:299:ASN:HB3	1:C:302:HIS:HB2	2.01	0.43
1:A:81:ARG:HH22	1:A:82:ARG:HH21	1.67	0.43
1:C:63:LEU:O	1:C:67:HIS:HB2	2.18	0.43
1:D:351:ARG:NH2	1:D:415:SER:O	2.51	0.43
1:B:1:ARG:CG	1:B:4:GLU:HB2	2.45	0.43
1:A:18:LEU:HD11	1:A:448:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:CG1	1:A:88:LEU:HD22	2.49	0.42
1:A:319:THR:HG22	1:A:322:ALA:N	2.14	0.42
1:A:89:TYR:CD1	1:A:123:TYR:HB2	2.54	0.42
1:A:323:GLY:O	1:A:327:VAL:HG23	2.18	0.42
1:B:194:ASP:OD1	1:B:196:ARG:HD3	2.19	0.42
1:D:143:GLU:N	1:D:144:PRO:CD	2.83	0.42
1:D:444:ALA:O	1:D:446:LEU:N	2.48	0.42
1:A:170:SER:HB3	1:A:233:THR:HG22	2.00	0.42
1:A:11:ALA:O	1:A:14:GLU:HB2	2.20	0.42
1:A:29:ASP:OD1	1:A:30:THR:N	2.53	0.42
1:A:45:LEU:HD22	1:A:438:ASN:HB2	2.00	0.42
1:B:30:THR:HB	1:B:430:GLU:O	2.19	0.42
1:D:95:ASP:OD2	1:D:284:SER:HB3	2.20	0.42
1:A:210:ILE:HG23	1:A:221:VAL:HG22	2.01	0.42
1:D:26:VAL:O	1:D:433:PHE:HA	2.19	0.42
1:C:39:ARG:HD3	5:C:714:HOH:O	2.20	0.41
1:D:50:ASN:O	1:D:53:LEU:HB2	2.20	0.41
1:D:15:ASP:HA	1:D:16:PRO:HD2	1.87	0.41
1:D:25:VAL:HG22	1:D:435:ILE:HG23	2.01	0.41
1:D:130:ASP:OD1	1:D:308:LYS:NZ	2.51	0.41
2:A:501:ZA3:C5	2:A:501:ZA3:O17	2.68	0.41
1:D:343:LEU:HD23	1:D:343:LEU:H	1.85	0.41
1:A:226:PRO:HB2	1:A:229:ALA:HB2	2.02	0.41
1:A:334:LEU:HD12	1:A:334:LEU:HA	1.90	0.41
1:B:385:GLU:O	1:B:391:GLY:HA3	2.20	0.41
1:C:437:ASN:C	1:C:438:ASN:HD22	2.24	0.41
1:B:61:GLU:HA	1:B:61:GLU:OE1	2.21	0.41
1:D:25:VAL:HA	1:D:434:SER:O	2.21	0.41
1:D:142:ASP:O	1:D:148:SER:HB3	2.21	0.41
1:B:299:ASN:HD22	1:B:302:HIS:H	1.58	0.40
1:B:397:ARG:HH22	1:B:449:GLN:NE2	2.17	0.40
1:D:464:ALA:HA	1:D:465:PRO:HD3	1.93	0.40
1:A:442:GLY:HA3	1:A:443:PRO:HD2	1.85	0.40
1:B:172:THR:HG22	1:B:231:PRO:CB	2.46	0.40
1:C:294:PHE:CD1	1:C:302:HIS:HB2	2.56	0.40
1:B:240:GLU:O	1:B:241:PRO:C	2.60	0.40
1:A:96:PRO:HB2	1:A:302:HIS:CD2	2.56	0.40
1:B:240:GLU:OE1	1:B:240:GLU:HA	2.21	0.40
1:C:206:ASN:OD1	1:C:206:ASN:C	2.60	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	464/466 (100%)	440 (95%)	22 (5%)	2 (0%)	34	54
1	B	464/466 (100%)	444 (96%)	19 (4%)	1 (0%)	47	68
1	C	464/466 (100%)	444 (96%)	18 (4%)	2 (0%)	34	54
1	D	464/466 (100%)	439 (95%)	24 (5%)	1 (0%)	47	68
All	All	1856/1864 (100%)	1767 (95%)	83 (4%)	6 (0%)	41	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	427	PRO
1	A	86	GLN
1	C	130	ASP
1	D	430	GLU
1	B	465	PRO
1	C	86	GLN

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	339/339 (100%)	317 (94%)	22 (6%)	17	33
1	B	338/339 (100%)	314 (93%)	24 (7%)	14	28
1	C	338/339 (100%)	318 (94%)	20 (6%)	19	37
1	D	339/339 (100%)	313 (92%)	26 (8%)	13	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1354/1356 (100%)	1262 (93%)	92 (7%)	16 30

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	39	ARG
1	A	46	LEU
1	A	82	ARG
1	A	88	LEU
1	A	98	LEU
1	A	116	ARG
1	A	136	ASP
1	A	154	LEU
1	A	170	SER
1	A	299	ASN
1	A	319	THR
1	A	320	TRP
1	A	324	LEU
1	A	349	LEU
1	A	375	THR
1	A	376	TRP
1	A	415	SER
1	A	438	ASN
1	A	441	SER
1	A	455	ARG
1	A	463	GLN
1	B	3	THR
1	B	4	GLU
1	B	18	LEU
1	B	30	THR
1	B	88	LEU
1	B	98	LEU
1	B	134	LEU
1	B	154	LEU
1	B	170	SER
1	B	198	VAL
1	B	259	THR
1	B	261	LYS
1	B	274	GLN
1	B	275	ASP
1	B	299	ASN

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Mol	Chain	Res	Type
1	B	302	HIS
1	B	324	LEU
1	B	329	GLU
1	B	349	LEU
1	B	369	SER
1	B	374	GLN
1	B	375	THR
1	B	386	SER
1	B	431	LEU
1	C	1	ARG
1	C	2	LEU
1	C	46	LEU
1	C	82	ARG
1	C	119	ARG
1	C	134	LEU
1	C	154	LEU
1	C	250	GLU
1	C	254	GLU
1	C	272	ASP
1	C	299	ASN
1	C	314	THR
1	C	320	TRP
1	C	324	LEU
1	C	349	LEU
1	C	376	TRP
1	C	377	SER
1	C	394	LEU
1	C	414	MET
1	C	431	LEU
1	D	2	LEU
1	D	3	THR
1	D	19	GLU
1	D	30	THR
1	D	63	LEU
1	D	66	ASP
1	D	77	SER
1	D	81	ARG
1	D	82	ARG
1	D	88	LEU
1	D	98	LEU
1	D	154	LEU
1	D	160	GLU

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Mol	Chain	Res	Type
1	D	184	LEU
1	D	214	VAL
1	D	281	ASP
1	D	291	LEU
1	D	299	ASN
1	D	320	TRP
1	D	324	LEU
1	D	343	LEU
1	D	349	LEU
1	D	375	THR
1	D	437	ASN
1	D	438	ASN
1	D	466	GLU

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	44	GLN
1	A	50	ASN
1	A	86	GLN
1	A	150	GLN
1	A	158	HIS
1	A	299	ASN
1	A	312	GLN
1	A	437	ASN
1	A	449	GLN
1	A	462	HIS
1	A	463	GLN
1	B	50	ASN
1	B	150	GLN
1	B	299	ASN
1	B	302	HIS
1	B	366	GLN
1	B	396	ASN
1	B	437	ASN
1	B	449	GLN
1	B	463	GLN
1	C	50	ASN
1	C	282	HIS
1	C	299	ASN
1	C	366	GLN
1	C	437	ASN

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Mol	Chain	Res	Type
1	C	449	GLN
1	D	44	GLN
1	D	50	ASN
1	D	150	GLN
1	D	158	HIS
1	D	299	ASN
1	D	302	HIS
1	D	437	ASN
1	D	449	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 4 are monoatomic - leaving 25 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	$\#\|Z\| > 2$
3	SO4	D	503	-	4,4,4	0.26	0	6,6,6	0.29	0
3	SO4	D	507	-	4,4,4	0.33	0	6,6,6	0.31	0
3	SO4	D	505	-	4,4,4	0.25	0	6,6,6	0.15	0
3	SO4	D	504	-	4,4,4	0.30	0	6,6,6	0.10	0
3	SO4	D	506	-	4,4,4	0.28	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	C	504	-	4,4,4	0.44	0	6,6,6	0.64	0
3	SO4	A	505	-	4,4,4	0.28	0	6,6,6	0.34	0
3	SO4	D	501	-	4,4,4	0.28	0	6,6,6	0.18	0
2	ZA3	D	502	1	15,16,17	2.90	2 (13%)	14,21,24	1.33	2 (14%)
3	SO4	C	506	-	4,4,4	0.29	0	6,6,6	0.18	0
2	ZA3	C	501	1	12,14,17	3.05	2 (16%)	15,18,24	1.25	3 (20%)
3	SO4	B	504	-	4,4,4	0.24	0	6,6,6	0.47	0
3	SO4	B	506	-	4,4,4	0.30	0	6,6,6	0.13	0
3	SO4	A	504	-	4,4,4	0.30	0	6,6,6	0.14	0
3	SO4	A	506	-	4,4,4	0.30	0	6,6,6	0.44	0
3	SO4	C	502	-	4,4,4	0.32	0	6,6,6	0.55	0
2	ZA3	B	501	1	12,14,17	3.05	2 (16%)	15,18,24	1.39	2 (13%)
3	SO4	B	502	-	4,4,4	0.41	0	6,6,6	0.36	0
3	SO4	A	502	-	4,4,4	0.31	0	6,6,6	0.20	0
3	SO4	C	505	-	4,4,4	0.31	0	6,6,6	0.23	0
3	SO4	B	505	-	4,4,4	0.33	0	6,6,6	0.24	0
3	SO4	C	503	-	4,4,4	0.19	0	6,6,6	0.21	0
3	SO4	B	503	-	4,4,4	0.27	0	6,6,6	0.32	0
3	SO4	A	503	-	4,4,4	0.34	0	6,6,6	0.85	0
2	ZA3	A	501	1	15,16,17	2.99	3 (20%)	14,21,24	1.35	3 (21%)

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	ZA3	C	501	1	-	6/10/11/14	0/1/1/1
2	ZA3	B	501	1	-	6/10/11/14	0/1/1/1
2	ZA3	A	501	1	-	6/10/13/14	0/1/1/1
2	ZA3	D	502	1	-	6/10/13/14	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ZA3	O17-N15	9.50	1.39	1.22
2	D	502	ZA3	O17-N15	9.28	1.39	1.22
2	B	501	ZA3	O17-N15	9.14	1.39	1.22
2	C	501	ZA3	O17-N15	8.82	1.38	1.22
2	C	501	ZA3	C14-N15	-5.29	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ZA3	C14-N15	-5.24	1.36	1.45
2	D	502	ZA3	C14-N15	-4.94	1.37	1.45
2	B	501	ZA3	C14-N15	-4.89	1.37	1.45
2	A	501	ZA3	B-C3	2.03	1.60	1.57

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	ZA3	C3-N4-C5	3.08	127.30	122.06
2	D	502	ZA3	C8-C7-C14	2.54	121.97	118.37
2	C	501	ZA3	C13-C14-N15	2.48	120.13	116.87
2	A	501	ZA3	O6-C5-C7	-2.43	116.58	121.03
2	D	502	ZA3	C8-C7-C5	-2.41	112.09	118.53
2	A	501	ZA3	C8-C7-C14	2.38	121.75	118.37
2	C	501	ZA3	C3-N4-C5	2.31	126.00	122.06
2	C	501	ZA3	O16-N15-C14	2.28	123.96	118.20
2	A	501	ZA3	C8-C7-C5	-2.23	112.57	118.53
2	B	501	ZA3	C7-C5-N4	2.02	121.25	117.32

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ZA3	C7-C14-N15-O16
2	B	501	ZA3	C7-C14-N15-O16
2	C	501	ZA3	C7-C14-N15-O16
2	D	502	ZA3	C7-C14-N15-O16
2	A	501	ZA3	O6-C5-C7-C14
2	D	502	ZA3	O6-C5-C7-C14
2	B	501	ZA3	O6-C5-C7-C14
2	C	501	ZA3	O6-C5-C7-C14
2	A	501	ZA3	O6-C5-C7-C8
2	C	501	ZA3	O6-C5-C7-C8
2	D	502	ZA3	O6-C5-C7-C8
2	B	501	ZA3	N4-C5-C7-C8
2	D	502	ZA3	N4-C5-C7-C8
2	A	501	ZA3	N4-C5-C7-C8
2	C	501	ZA3	N4-C5-C7-C8
2	B	501	ZA3	O6-C5-C7-C8
2	A	501	ZA3	N4-C5-C7-C14
2	D	502	ZA3	N4-C5-C7-C14
2	B	501	ZA3	N4-C5-C7-C14

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Mol	Chain	Res	Type	Atoms
2	C	501	ZA3	N4-C5-C7-C14
2	A	501	ZA3	C13-C14-N15-O16
2	B	501	ZA3	C13-C14-N15-O16
2	C	501	ZA3	C13-C14-N15-O16
2	D	502	ZA3	C13-C14-N15-O16

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	SO4	3	0
2	D	502	ZA3	2	0
2	C	501	ZA3	3	0
3	A	506	SO4	1	0
2	B	501	ZA3	3	0
3	C	503	SO4	1	0
2	A	501	ZA3	3	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, 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	466/466 (100%)	-0.24	3 (0%)	89	90	20, 33, 56, 81	0
1	B	466/466 (100%)	-0.31	5 (1%)	80	82	20, 35, 61, 113	0
1	C	466/466 (100%)	-0.28	3 (0%)	89	90	21, 33, 53, 87	0
1	D	466/466 (100%)	-0.02	11 (2%)	59	62	22, 47, 79, 96	0
All	All	1864/1864 (100%)	-0.21	22 (1%)	79	80	20, 36, 68, 113	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	LEU	4.9
1	D	262	GLY	3.9
1	D	429	GLY	3.5
1	A	429	GLY	3.4
1	B	2	LEU	3.1
1	D	118	VAL	3.1
1	B	275	ASP	2.8
1	A	80	GLY	2.8
1	D	261	LYS	2.7
1	C	428	GLU	2.6
1	C	3	THR	2.5
1	D	264	VAL	2.4
1	D	260	VAL	2.4
1	D	78	ALA	2.3
1	B	428	GLU	2.3
1	D	400	GLY	2.2
1	B	426	GLY	2.2
1	D	399	ARG	2.2
1	D	80	GLY	2.2
1	D	84	GLU	2.1
1	A	259	THR	2.1
1	B	1	ARG	2.1

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, 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	B-factors(Å^2)	Q<0.9
4	MG	A	508	1/1	0.76	0.22	60,60,60,60	0
3	SO4	A	506	5/5	0.80	0.22	87,87,87,88	0
2	ZA3	D	502	16/17	0.90	0.20	49,60,63,63	0
4	MG	D	509	1/1	0.90	0.08	48,48,48,48	0
3	SO4	D	501	5/5	0.91	0.22	77,77,78,78	0
3	SO4	D	507	5/5	0.92	0.13	83,83,83,84	0
2	ZA3	A	501	16/17	0.93	0.16	32,44,47,48	0
3	SO4	A	504	5/5	0.94	0.11	79,79,79,80	0
3	SO4	C	506	5/5	0.95	0.14	71,72,73,73	0
3	SO4	B	505	5/5	0.95	0.13	77,78,78,78	0
3	SO4	D	504	5/5	0.95	0.11	74,74,75,75	0
3	SO4	B	506	5/5	0.95	0.12	59,59,60,61	0
3	SO4	C	503	5/5	0.95	0.12	62,64,64,64	0
4	MG	D	508	1/1	0.95	0.12	47,47,47,47	0
3	SO4	C	505	5/5	0.95	0.13	74,74,75,75	0
2	ZA3	B	501	14/17	0.96	0.14	20,31,33,33	0
3	SO4	B	503	5/5	0.96	0.14	66,66,67,67	0
3	SO4	D	503	5/5	0.96	0.19	60,62,63,63	0
2	ZA3	C	501	14/17	0.96	0.14	18,28,30,33	0
3	SO4	D	505	5/5	0.97	0.08	75,75,76,76	0
4	MG	A	507	1/1	0.98	0.09	27,27,27,27	0
3	SO4	C	502	5/5	0.98	0.08	38,38,40,42	0
3	SO4	A	502	5/5	0.98	0.14	51,53,54,56	0
3	SO4	A	505	5/5	0.98	0.11	54,55,57,57	0
3	SO4	B	502	5/5	0.99	0.07	41,42,44,46	0
3	SO4	C	504	5/5	0.99	0.09	33,35,36,37	0
3	SO4	A	503	5/5	0.99	0.09	31,32,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	504	5/5	0.99	0.13	35,36,38,39	0
3	SO4	D	506	5/5	0.99	0.12	41,42,42,43	0

6.5 Other polymers (i)

There are no such residues in this entry.