Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:50 PM UTC

PDB ID	:	2WKE / pdb_00002wke
Title	:	Crystal structure of the Actinomadura R39 DD-peptidase inhibited by 6- bet a-iodopenicillanate.
Authors	:	Sauvage, E.; Herman, R.; Kerff, F.; Charlier, P.
Deposited on	:	2009-06-10
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

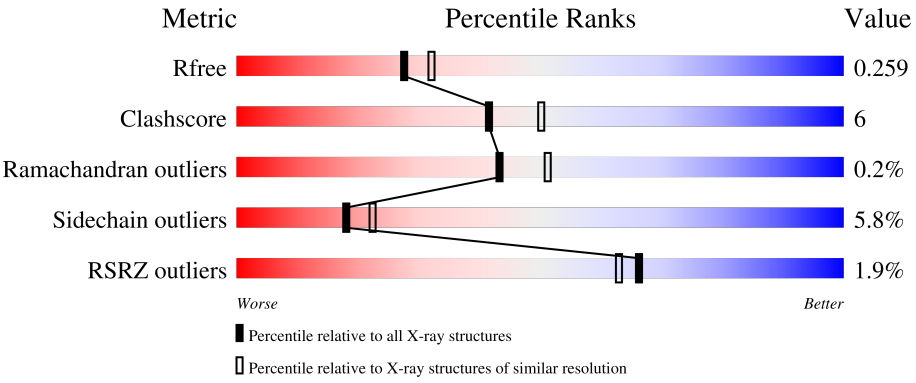
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	3% 86% 13%
1	B	466	% 85% 14%
1	C	466	% 87% 12%
1	D	466	3% 85% 14%

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	A	605	-	-	X	-
3	SO4	B	605	-	-	X	-
3	SO4	C	605	-	-	X	-
3	SO4	D	605	-	-	X	-

2 Entry composition (i)

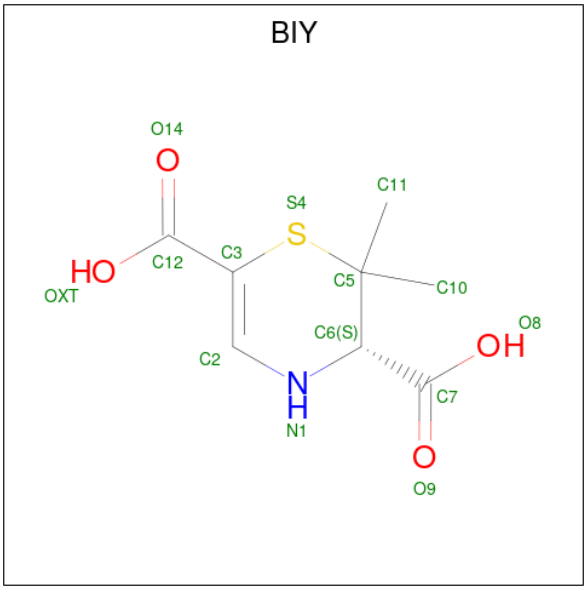
There are 5 unique types of molecules in this entry. The entry contains 14160 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	466	Total	C	N	O	S	0	0	0
			3353	2076	564	707	6			
1	B	466	Total	C	N	O	S	0	0	1
			3344	2071	564	703	6			
1	C	466	Total	C	N	O	S	0	0	1
			3344	2071	564	703	6			
1	D	466	Total	C	N	O	S	0	0	0
			3353	2076	564	707	6			

- Molecule 2 is (3S)-2,2-dimethyl-3,4-dihydro-2H-1,4-thiazine-3,6-dicarboxylic acid (CCD ID: BIY) (formula: $C_8H_{11}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

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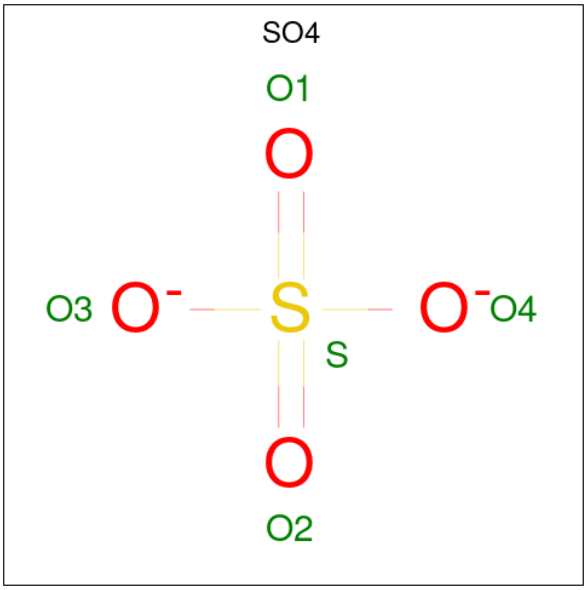
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O S 13 8 1 3 1	0	0
2	D	1	Total C N O S 13 8 1 3 1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 4 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Co 4 4	0	0
4	B	3	Total Co 3 3	0	0
4	C	3	Total Co 3 3	0	0
4	D	4	Total Co 4 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	170	Total O 170 170	0	0
5	B	143	Total O 143 143	0	0

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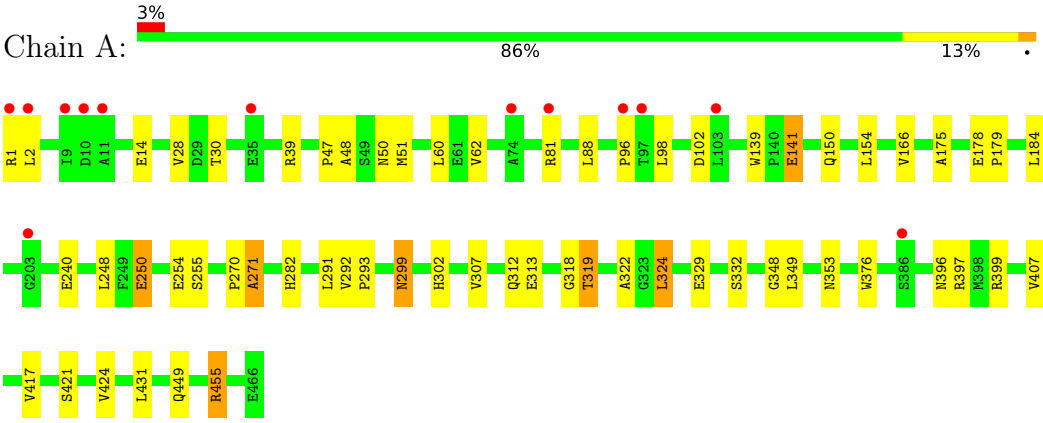
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	148	Total O 148 148	0	0
5	D	139	Total O 139 139	0	0

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.

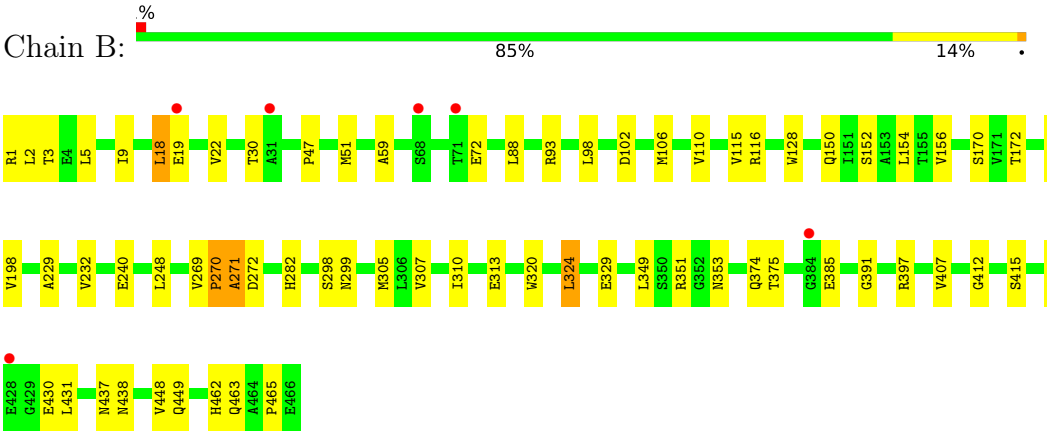
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain A:



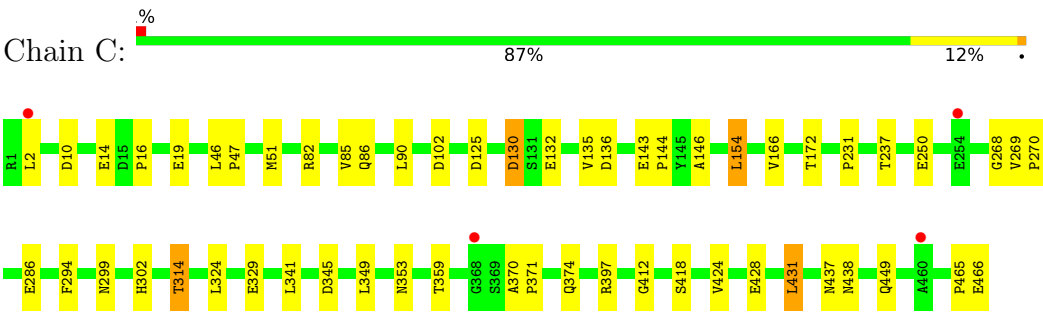
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain B:



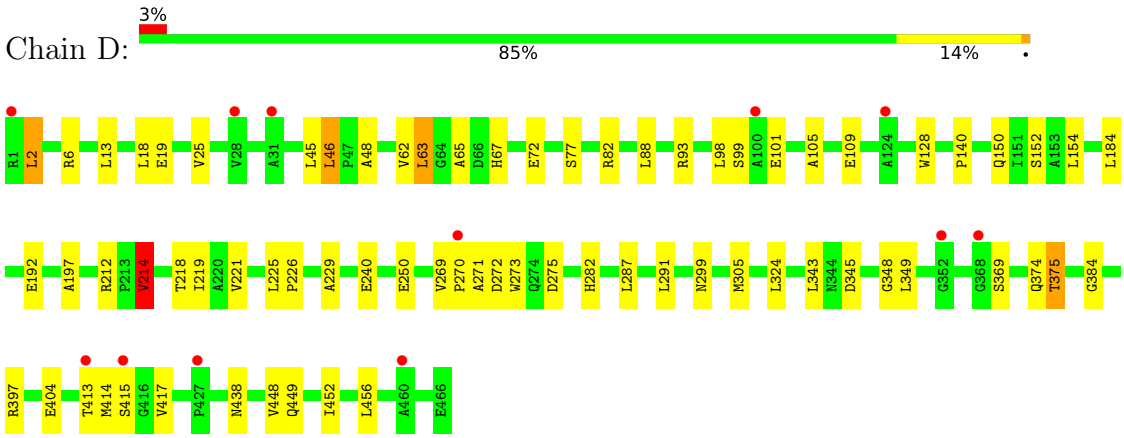
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.98Å 92.69Å 107.13Å 90.00° 95.03° 90.00°	Depositor
Resolution (Å)	29.06 – 2.20 29.06 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.5 (29.06-2.20) 91.5 (29.06-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.261 0.206 , 0.259	Depositor DCC
R_{free} test set	4728 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å^2)	33.8	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 32.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14160	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.71	0/3412	0.92	1/4666 (0.0%)
1	B	0.71	2/3403 (0.1%)	0.91	3/4656 (0.1%)
1	C	0.68	1/3403 (0.0%)	0.90	2/4656 (0.0%)
1	D	0.67	0/3412	0.91	3/4666 (0.1%)
All	All	0.69	3/13630 (0.0%)	0.91	9/18644 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	462	HIS	CE1-NE2	7.07	1.39	1.32
1	C	465	PRO	C-N	-6.52	1.24	1.33
1	B	465	PRO	C-N	-6.29	1.24	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	269	VAL	CA-C-N	7.11	128.73	119.84
1	B	269	VAL	C-N-CA	7.11	128.73	119.84
1	D	269	VAL	CA-C-N	6.49	127.00	119.47
1	D	269	VAL	C-N-CA	6.49	127.00	119.47
1	C	269	VAL	CA-C-N	5.90	127.21	119.84
1	C	269	VAL	C-N-CA	5.90	127.21	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	116	ARG	N-CA-C	-5.88	106.65	113.88
1	D	214	VAL	CB-CA-C	-5.34	102.62	111.32
1	A	409	ALA	N-CA-C	5.09	116.99	108.99

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	GLY	Peptide

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	46	0
1	B	3344	0	3194	44	0
1	C	3344	0	3194	39	0
1	D	3353	0	3200	40	0
2	A	13	0	9	1	0
2	B	13	0	9	1	0
2	C	13	0	9	0	0
2	D	13	0	9	0	0
3	A	25	0	0	3	0
3	B	25	0	0	6	0
3	C	25	0	0	6	0
3	D	25	0	0	3	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	4	0	0	0	0
5	A	170	0	0	11	0
5	B	143	0	0	4	0
5	C	148	0	0	9	0
5	D	139	0	0	8	0
All	All	14160	0	12824	169	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 6.

All (169) 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:C:166:VAL:HG12	5:C:2101:HOH:O	1.23	1.38
1:D:282:HIS:NE2	3:D:605:SO4:O4	1.88	1.06
1:A:282:HIS:NE2	3:A:605:SO4:O1	1.98	0.95
1:B:51:MET:CE	1:B:353:ASN:HB3	1.97	0.93
1:B:282:HIS:NE2	3:B:605:SO4:O3	2.09	0.86
1:D:287:LEU:HB3	5:D:2009:HOH:O	1.75	0.86
1:A:319:THR:HG21	5:A:2127:HOH:O	1.77	0.85
1:A:270:PRO:O	1:A:271:ALA:HB3	1.77	0.83
1:B:51:MET:HE3	1:B:353:ASN:CG	2.04	0.82
1:C:102:ASP:OD2	3:C:605:SO4:O3	1.97	0.82
1:B:51:MET:HE3	1:B:353:ASN:HB3	1.60	0.82
1:A:1:ARG:HH22	1:A:455:ARG:HH22	1.28	0.81
1:B:102:ASP:OD2	3:B:605:SO4:O3	1.99	0.81
1:C:282:HIS:NE2	3:C:605:SO4:O3	2.14	0.81
1:B:51:MET:HE3	1:B:353:ASN:CB	2.14	0.78
1:C:237:THR:HG22	5:C:2101:HOH:O	1.83	0.77
1:C:16:PRO:HA	1:C:19:GLU:OE2	1.86	0.76
1:A:319:THR:HG22	1:A:322:ALA:H	1.50	0.75
1:A:51:MET:HE2	1:A:353:ASN:HB3	1.69	0.74
1:C:374:GLN:HG2	5:D:2091:HOH:O	1.88	0.74
1:A:270:PRO:O	1:A:271:ALA:CB	2.35	0.73
1:C:282:HIS:NE2	3:C:605:SO4:S	2.61	0.73
1:A:166:VAL:HG12	5:A:2097:HOH:O	1.90	0.72
1:A:150:GLN:HE22	1:A:240:GLU:H	1.38	0.71
1:D:150:GLN:NE2	1:D:240:GLU:H	1.88	0.71
1:A:51:MET:CE	1:A:353:ASN:HB3	2.21	0.70
1:D:282:HIS:CD2	3:D:605:SO4:O4	2.43	0.70
1:D:282:HIS:NE2	3:D:605:SO4:S	2.56	0.70
1:D:150:GLN:HE22	1:D:240:GLU:H	1.38	0.68
1:A:178:GLU:HG3	1:A:179:PRO:HD2	1.75	0.67
1:B:282:HIS:NE2	3:B:605:SO4:S	2.62	0.67
1:B:351:ARG:NH2	1:B:415:SER:O	2.28	0.66
1:C:166:VAL:CG1	5:C:2101:HOH:O	2.04	0.66
1:A:1:ARG:HG3	5:A:2002:HOH:O	1.94	0.66
1:B:229:ALA:O	5:B:2088:HOH:O	2.14	0.66
1:B:150:GLN:HE22	1:B:240:GLU:H	1.43	0.65
1:C:397:ARG:HH12	1:C:449:GLN:HE21	1.44	0.65
1:A:102:ASP:OD1	3:A:605:SO4:O1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ASP:CG	3:C:605:SO4:O3	2.39	0.65
1:B:150:GLN:NE2	1:B:240:GLU:H	1.94	0.65
1:B:270:PRO:O	1:B:271:ALA:CB	2.45	0.64
1:C:172:THR:HG22	1:C:231:PRO:HB3	1.79	0.64
1:C:237:THR:CG2	5:C:2101:HOH:O	2.43	0.63
1:D:77:SER:HB2	5:D:2014:HOH:O	1.98	0.62
1:A:1:ARG:HH22	1:A:455:ARG:NH2	1.95	0.62
1:C:102:ASP:OD2	3:C:605:SO4:S	2.57	0.62
1:B:375:THR:HG23	5:B:2119:HOH:O	1.98	0.62
1:A:139:TRP:HB3	1:A:141:GLU:OE1	2.00	0.61
1:A:150:GLN:NE2	1:A:240:GLU:H	1.99	0.60
1:D:384:GLY:HA3	1:D:404:GLU:HG3	1.83	0.60
1:B:152:SER:O	1:B:305:MET:HE3	2.01	0.60
1:C:270:PRO:O	1:C:271:ALA:CB	2.50	0.60
1:D:99:SER:OG	1:D:101:GLU:HG2	2.00	0.60
1:B:59:ALA:HA	1:B:310:ILE:HD11	1.83	0.60
1:B:397:ARG:HH12	1:B:449:GLN:HE21	1.48	0.60
1:B:270:PRO:O	1:B:271:ALA:HB3	2.02	0.59
1:C:282:HIS:CE1	3:C:605:SO4:O3	2.56	0.59
1:D:270:PRO:O	1:D:271:ALA:HB3	2.01	0.59
1:B:51:MET:HE1	1:B:353:ASN:HB3	1.82	0.59
1:C:130:ASP:HB3	1:C:132:GLU:H	1.67	0.58
1:C:397:ARG:HH12	1:C:449:GLN:NE2	2.02	0.57
1:C:47:PRO:HG3	1:C:51:MET:CE	2.35	0.56
1:C:270:PRO:O	1:C:271:ALA:HB3	2.05	0.56
1:B:102:ASP:OD2	3:B:605:SO4:S	2.63	0.56
1:D:67:HIS:N	5:D:2009:HOH:O	2.39	0.55
1:A:1:ARG:NH2	1:A:455:ARG:HH22	1.99	0.55
1:A:141:GLU:HG2	5:A:2059:HOH:O	2.05	0.55
1:D:197:ALA:HB2	1:D:221:VAL:HG12	1.88	0.55
1:A:102:ASP:OD1	3:A:605:SO4:S	2.64	0.55
1:D:6:ARG:HD3	5:D:2002:HOH:O	2.07	0.55
1:A:141:GLU:CG	5:A:2059:HOH:O	2.56	0.53
1:A:319:THR:CG2	1:A:322:ALA:H	2.20	0.53
1:D:72:GLU:OE1	1:D:93:ARG:NH2	2.41	0.52
1:A:166:VAL:CG1	5:A:2097:HOH:O	2.55	0.52
1:A:250:GLU:HG2	5:A:2103:HOH:O	2.10	0.52
1:B:47:PRO:HG3	1:B:51:MET:HE2	1.92	0.50
1:B:47:PRO:CG	1:B:51:MET:HE2	2.41	0.50
1:C:370:ALA:HB1	1:C:371:PRO:HD2	1.92	0.50
1:A:299:ASN:ND2	1:A:302:HIS:H	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:PRO:HG3	1:C:51:MET:HE2	1.94	0.49
2:B:500:BIY:H103	2:B:500:BIY:C2	2.43	0.48
1:B:407:VAL:HG22	1:B:424:VAL:HG22	1.95	0.48
1:C:51:MET:HE3	1:C:353:ASN:HB3	1.95	0.48
1:D:48:ALA:O	1:D:348:GLY:HA3	2.13	0.48
1:C:286:GLU:HG3	5:C:2107:HOH:O	2.13	0.48
1:B:102:ASP:CG	3:B:605:SO4:O3	2.56	0.48
1:A:271:ALA:HA	5:A:2109:HOH:O	2.14	0.48
1:B:282:HIS:CD2	3:B:605:SO4:O3	2.67	0.48
1:B:93:ARG:HD3	1:B:128:TRP:CE3	2.49	0.47
1:C:90:LEU:HG	1:C:154:LEU:HD11	1.96	0.47
1:C:85:VAL:HG12	1:C:86:GLN:N	2.29	0.47
1:D:271:ALA:C	1:D:273:TRP:H	2.22	0.47
1:D:140:PRO:HB3	1:D:214:VAL:HG11	1.97	0.47
1:D:225:LEU:HD12	1:D:226:PRO:HD2	1.97	0.47
1:B:18:LEU:CD2	1:B:448:VAL:HG11	2.45	0.47
1:C:135:VAL:HG21	1:C:345:ASP:HB3	1.97	0.47
1:D:452:ILE:O	1:D:456:LEU:HG	2.14	0.47
1:A:81:ARG:HD3	1:B:313:GLU:OE1	2.14	0.47
1:C:437:ASN:C	1:C:438:ASN:HD22	2.23	0.47
1:D:18:LEU:HD11	1:D:448:VAL:HG11	1.96	0.47
1:A:397:ARG:HH12	1:A:449:GLN:HE21	1.63	0.47
1:C:466:GLU:N	5:C:2144:HOH:O	2.48	0.47
1:D:287:LEU:CB	5:D:2009:HOH:O	2.48	0.47
1:B:5:LEU:O	1:B:9:ILE:HG13	2.14	0.47
1:C:46:LEU:CD2	5:C:2120:HOH:O	2.63	0.46
1:D:414:MET:HG2	1:D:417:VAL:HB	1.97	0.46
2:A:500:BIY:H103	2:A:500:BIY:O9	2.15	0.46
1:A:60:LEU:HD11	1:A:291:LEU:HD11	1.97	0.46
1:C:424:VAL:HB	1:C:431:LEU:HB2	1.97	0.46
1:A:299:ASN:C	1:A:299:ASN:HD22	2.24	0.46
1:D:345:ASP:OD1	1:D:345:ASP:C	2.59	0.46
1:B:424:VAL:HB	1:B:431:LEU:HB2	1.98	0.46
1:A:184:LEU:HB2	1:A:188:GLU:HG2	1.98	0.46
1:B:156:VAL:HG21	1:B:248:LEU:HD12	1.97	0.46
1:D:397:ARG:HH12	1:D:449:GLN:HE21	1.63	0.45
1:D:45:LEU:HD22	1:D:438:ASN:HB2	1.97	0.45
1:B:1:ARG:HD2	1:D:2:LEU:HG	1.98	0.45
1:C:314:THR:CB	5:C:2111:HOH:O	2.64	0.45
1:B:385:GLU:O	1:B:391:GLY:HA3	2.15	0.45
1:B:110:VAL:HG12	1:B:115:VAL:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PRO:HB2	1:A:302:HIS:CD2	2.52	0.45
1:B:72:GLU:HG2	5:B:2026:HOH:O	2.17	0.45
1:B:397:ARG:HH12	1:B:449:GLN:NE2	2.14	0.45
1:C:294:PHE:HB2	1:C:302:HIS:HD2	1.81	0.45
1:B:307:VAL:HG11	1:B:324:LEU:HD13	1.99	0.45
1:A:47:PRO:HD2	5:A:2134:HOH:O	2.17	0.44
1:B:194:ASP:OD2	1:B:196:ARG:HD3	2.16	0.44
1:A:396:ASN:OD1	1:A:399:ARG:NH1	2.51	0.44
1:A:186:ALA:HB1	1:A:248:LEU:HD11	2.00	0.44
1:C:397:ARG:NH1	1:C:449:GLN:HE21	2.13	0.44
1:C:125:ASP:CG	1:C:268:GLY:HA2	2.42	0.44
1:D:270:PRO:O	1:D:271:ALA:CB	2.66	0.44
1:C:146:ALA:HA	5:C:2101:HOH:O	2.18	0.44
1:D:192:GLU:HG3	1:D:218:THR:OG1	2.17	0.44
1:D:226:PRO:HG2	1:D:229:ALA:HB2	1.99	0.44
1:A:307:VAL:HG11	1:A:324:LEU:HD13	1.99	0.44
1:A:407:VAL:HG22	1:A:424:VAL:HG22	2.00	0.44
1:B:437:ASN:C	1:B:438:ASN:HD22	2.25	0.44
1:D:152:SER:O	1:D:305:MET:HE3	2.17	0.43
1:B:51:MET:CE	1:B:353:ASN:CB	2.77	0.43
1:C:143:GLU:N	1:C:144:PRO:CD	2.82	0.43
1:B:320:TRP:O	1:B:324:LEU:HB2	2.19	0.43
1:C:10:ASP:O	1:C:14:GLU:HG2	2.19	0.43
1:C:412:GLY:O	1:C:418:SER:HA	2.19	0.43
1:B:170:SER:HA	1:B:232:VAL:O	2.19	0.43
1:D:13:LEU:HD11	1:D:25:VAL:HG21	2.00	0.42
1:D:397:ARG:NH1	1:D:449:GLN:HE21	2.16	0.42
1:A:1:ARG:HH12	1:A:455:ARG:HH12	1.65	0.42
1:A:51:MET:HE3	1:A:353:ASN:OD1	2.20	0.42
1:D:93:ARG:HG2	1:D:128:TRP:CD2	2.54	0.42
1:A:414:MET:HB2	1:A:417:VAL:HB	2.01	0.42
1:B:106:MET:O	1:B:110:VAL:HG23	2.20	0.42
1:D:212:ARG:HB2	1:D:219:ILE:HD13	2.01	0.42
1:D:397:ARG:HH12	1:D:449:GLN:NE2	2.18	0.42
1:A:175:ALA:HB3	5:A:2085:HOH:O	2.20	0.42
1:D:105:ALA:O	1:D:109:GLU:HG3	2.20	0.42
1:D:65:ALA:C	5:D:2009:HOH:O	2.63	0.41
1:A:292:VAL:HB	1:A:293:PRO:CD	2.50	0.41
1:D:375:THR:HG23	5:D:2117:HOH:O	2.19	0.41
1:A:51:MET:HE3	1:A:353:ASN:CG	2.45	0.41
1:D:62:VAL:HG12	1:D:63:LEU:HD13	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:LEU:HG	1:C:359:THR:HG21	2.02	0.41
1:D:46:LEU:N	1:D:46:LEU:HD23	2.36	0.41
1:B:412:GLY:O	1:B:418:SER:HA	2.20	0.41
1:A:271:ALA:HB2	5:A:2034:HOH:O	2.21	0.41
1:A:62:VAL:HG12	1:A:313:GLU:HG2	2.03	0.40
1:A:48:ALA:O	1:A:348:GLY:HA3	2.21	0.40
1:A:50:ASN:ND2	1:A:421:SER:OG	2.55	0.40
1:B:172:THR:HB	5:B:2019:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	464/466 (100%)	450 (97%)	13 (3%)	1 (0%)	43	51
1	B	464/466 (100%)	444 (96%)	19 (4%)	1 (0%)	43	51
1	C	464/466 (100%)	444 (96%)	18 (4%)	2 (0%)	30	34
1	D	464/466 (100%)	447 (96%)	17 (4%)	0	100	100
All	All	1856/1864 (100%)	1785 (96%)	67 (4%)	4 (0%)	43	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	271	ALA
1	C	271	ALA
1	C	130	ASP
1	A	271	ALA

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%)	15	18
1	B	338/339 (100%)	318 (94%)	20 (6%)	18	22
1	C	338/339 (100%)	325 (96%)	13 (4%)	29	40
1	D	339/339 (100%)	316 (93%)	23 (7%)	14	17
All	All	1354/1356 (100%)	1276 (94%)	78 (6%)	18	22

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	14	GLU
1	A	28	VAL
1	A	30	THR
1	A	39	ARG
1	A	88	LEU
1	A	98	LEU
1	A	141	GLU
1	A	154	LEU
1	A	250	GLU
1	A	254	GLU
1	A	255	SER
1	A	299	ASN
1	A	312	GLN
1	A	319	THR
1	A	324	LEU
1	A	329	GLU
1	A	332	SER
1	A	349	LEU
1	A	376	TRP
1	A	431	LEU
1	A	455	ARG
1	B	2	LEU
1	B	3	THR

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Mol	Chain	Res	Type
1	B	18	LEU
1	B	19	GLU
1	B	22	VAL
1	B	30	THR
1	B	88	LEU
1	B	98	LEU
1	B	154	LEU
1	B	198	VAL
1	B	270	PRO
1	B	272	ASP
1	B	298	SER
1	B	299	ASN
1	B	324	LEU
1	B	329	GLU
1	B	349	LEU
1	B	374	GLN
1	B	430	GLU
1	B	463	GLN
1	C	2	LEU
1	C	82	ARG
1	C	136	ASP
1	C	154	LEU
1	C	250	GLU
1	C	272	ASP
1	C	299	ASN
1	C	314	THR
1	C	324	LEU
1	C	329	GLU
1	C	349	LEU
1	C	428	GLU
1	C	431	LEU
1	D	2	LEU
1	D	19	GLU
1	D	46	LEU
1	D	63	LEU
1	D	82	ARG
1	D	88	LEU
1	D	98	LEU
1	D	154	LEU
1	D	184	LEU
1	D	214	VAL
1	D	250	GLU

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Mol	Chain	Res	Type
1	D	272	ASP
1	D	275	ASP
1	D	291	LEU
1	D	299	ASN
1	D	324	LEU
1	D	343	LEU
1	D	349	LEU
1	D	369	SER
1	D	374	GLN
1	D	375	THR
1	D	413	THR
1	D	415	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	150	GLN
1	A	299	ASN
1	A	312	GLN
1	A	437	ASN
1	A	449	GLN
1	A	463	GLN
1	B	50	ASN
1	B	150	GLN
1	B	299	ASN
1	B	396	ASN
1	B	437	ASN
1	B	449	GLN
1	C	50	ASN
1	C	299	ASN
1	C	437	ASN
1	C	449	GLN
1	D	44	GLN
1	D	50	ASN
1	D	150	GLN
1	D	299	ASN
1	D	302	HIS
1	D	366	GLN
1	D	396	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 14 are monoatomic - leaving 24 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	A	601	-	4,4,4	0.33	0	6,6,6	0.42	0
2	BIY	C	500	1	11,13,14	3.30	6 (54%)	11,19,21	2.59	4 (36%)
3	SO4	A	602	-	4,4,4	0.26	0	6,6,6	0.15	0
3	SO4	D	601	-	4,4,4	0.23	0	6,6,6	0.25	0
2	BIY	A	500	1	11,13,14	3.26	4 (36%)	11,19,21	2.57	4 (36%)
3	SO4	B	602	-	4,4,4	0.25	0	6,6,6	0.20	0
3	SO4	B	603	-	4,4,4	0.25	0	6,6,6	0.22	0
3	SO4	B	605	-	4,4,4	0.44	0	6,6,6	0.45	0
3	SO4	D	603	-	4,4,4	0.37	0	6,6,6	0.95	1 (16%)
3	SO4	A	604	-	4,4,4	0.20	0	6,6,6	0.23	0
3	SO4	B	604	-	4,4,4	0.25	0	6,6,6	0.20	0
3	SO4	B	601	-	4,4,4	0.23	0	6,6,6	0.35	0
3	SO4	C	605	-	4,4,4	0.61	0	6,6,6	0.36	0
3	SO4	A	603	-	4,4,4	0.24	0	6,6,6	0.41	0
2	BIY	B	500	1	11,13,14	3.48	6 (54%)	11,19,21	2.28	3 (27%)
2	BIY	D	500	1	11,13,14	4.41	5 (45%)	11,19,21	2.55	5 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	C	601	-	4,4,4	0.19	0	6,6,6	0.38	0
3	SO4	D	604	-	4,4,4	0.25	0	6,6,6	0.46	0
3	SO4	D	602	-	4,4,4	0.23	0	6,6,6	0.19	0
3	SO4	C	602	-	4,4,4	0.20	0	6,6,6	0.22	0
3	SO4	C	604	-	4,4,4	0.22	0	6,6,6	0.34	0
3	SO4	D	605	-	4,4,4	0.42	0	6,6,6	0.26	0
3	SO4	C	603	-	4,4,4	0.23	0	6,6,6	0.13	0
3	SO4	A	605	-	4,4,4	0.77	0	6,6,6	0.60	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	BIY	C	500	1	-	0/3/22/24	0/1/1/1
2	BIY	B	500	1	-	0/3/22/24	0/1/1/1
2	BIY	D	500	1	-	1/3/22/24	0/1/1/1
2	BIY	A	500	1	-	0/3/22/24	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	BIY	C2-N1	10.84	1.51	1.34
2	C	500	BIY	C5-S4	-8.31	1.78	1.84
2	D	500	BIY	C5-S4	-7.47	1.78	1.84
2	B	500	BIY	C5-S4	-7.26	1.78	1.84
2	A	500	BIY	C5-S4	-6.82	1.79	1.84
2	B	500	BIY	C2-N1	6.62	1.44	1.34
2	A	500	BIY	C2-N1	6.60	1.44	1.34
2	D	500	BIY	C6-N1	4.10	1.51	1.45
2	B	500	BIY	C6-N1	4.01	1.50	1.45
2	C	500	BIY	C6-N1	3.56	1.50	1.45
2	C	500	BIY	C2-N1	3.50	1.39	1.34
2	A	500	BIY	C6-N1	3.34	1.50	1.45
2	D	500	BIY	C12-C3	3.34	1.49	1.45
2	C	500	BIY	C2-C3	-2.97	1.30	1.35
2	B	500	BIY	C3-S4	-2.82	1.67	1.73
2	C	500	BIY	C3-S4	-2.54	1.67	1.73
2	A	500	BIY	C3-S4	-2.40	1.68	1.73
2	C	500	BIY	C12-C3	2.28	1.48	1.45
2	D	500	BIY	C3-S4	-2.14	1.68	1.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	BIY	C2-C3	-2.14	1.32	1.35
2	B	500	BIY	C12-C3	2.11	1.48	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	BIY	C7-C6-N1	5.73	119.27	108.74
2	B	500	BIY	C5-C6-N1	5.61	115.56	109.51
2	A	500	BIY	O14-C12-C3	-5.54	115.20	124.98
2	C	500	BIY	C5-C6-N1	5.45	115.39	109.51
2	C	500	BIY	C12-C3-S4	4.78	124.76	112.53
2	A	500	BIY	C7-C6-N1	4.42	116.87	108.74
2	D	500	BIY	C12-C3-S4	3.67	121.93	112.53
2	B	500	BIY	C12-C3-S4	3.67	121.91	112.53
2	C	500	BIY	O14-C12-C3	-3.39	119.00	124.98
2	A	500	BIY	C10-C5-C11	-2.90	106.27	109.64
2	D	500	BIY	C10-C5-C11	-2.90	106.28	109.64
2	A	500	BIY	C12-C3-S4	2.84	119.80	112.53
2	C	500	BIY	C10-C5-C11	-2.47	106.77	109.64
2	D	500	BIY	C11-C5-S4	2.36	114.07	107.56
2	B	500	BIY	O14-C12-C3	-2.15	121.20	124.98
2	D	500	BIY	O14-C12-C3	-2.13	121.22	124.98
3	D	603	SO4	O3-S-O1	2.04	120.20	109.56

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	500	BIY	N1-C6-C7-O9

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	BIY	1	0
3	B	605	SO4	6	0
3	C	605	SO4	6	0
2	B	500	BIY	1	0
3	D	605	SO4	3	0
3	A	605	SO4	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

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	466/466 (100%)	0.16	13 (2%)	55	52	11, 19, 27, 32	0
1	B	466/466 (100%)	0.07	6 (1%)	75	73	13, 21, 29, 35	0
1	C	466/466 (100%)	-0.04	4 (0%)	81	79	11, 19, 27, 33	0
1	D	466/466 (100%)	0.35	12 (2%)	57	54	9, 23, 34, 39	0
All	All	1864/1864 (100%)	0.13	35 (1%)	66	63	9, 20, 31, 39	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	368	GLY	3.8
1	A	74	ALA	3.8
1	C	460	ALA	3.4
1	B	428	GLU	3.3
1	A	1	ARG	3.1
1	A	35	GLU	3.0
1	C	2	LEU	3.0
1	D	100	ALA	2.9
1	B	19	GLU	2.9
1	A	97	THR	2.9
1	D	415	SER	2.8
1	D	1	ARG	2.8
1	D	427	PRO	2.8
1	D	31	ALA	2.8
1	D	28	VAL	2.7
1	A	9	ILE	2.7
1	D	368	GLY	2.7
1	A	103	LEU	2.7
1	D	460	ALA	2.5
1	D	413	THR	2.4
1	A	203	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	124	ALA	2.4
1	A	96	PRO	2.3
1	D	270	PRO	2.3
1	B	68	SER	2.3
1	C	254	GLU	2.3
1	A	2	LEU	2.2
1	B	384	GLY	2.2
1	D	352	GLY	2.2
1	A	10	ASP	2.1
1	B	71	THR	2.1
1	A	81	ARG	2.1
1	A	386	SER	2.0
1	A	11	ALA	2.0
1	B	31	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no oligosaccharides 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
3	SO4	A	604	5/5	0.77	0.15	70,71,72,72	0
3	SO4	A	603	5/5	0.81	0.23	56,57,59,59	0
4	CO	B	613	1/1	0.85	0.11	97,97,97,97	0
3	SO4	D	602	5/5	0.87	0.20	66,66,66,67	0
2	BIY	D	500	13/14	0.87	0.12	26,37,39,40	0
4	CO	D	613	1/1	0.87	0.10	87,87,87,87	0
3	SO4	B	602	5/5	0.88	0.12	55,55,56,57	0
3	SO4	A	602	5/5	0.88	0.20	63,64,65,65	0
3	SO4	C	603	5/5	0.90	0.19	60,60,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BIY	A	500	13/14	0.90	0.10	29,37,42,45	0
4	CO	C	612	1/1	0.91	0.08	67,67,67,67	0
3	SO4	C	602	5/5	0.91	0.13	52,52,54,54	0
4	CO	A	613	1/1	0.92	0.08	62,62,62,62	0
2	BIY	C	500	13/14	0.92	0.09	32,35,39,39	0
3	SO4	A	605	5/5	0.92	0.12	17,25,27,29	0
2	BIY	B	500	13/14	0.92	0.10	32,37,37,37	0
3	SO4	D	601	5/5	0.93	0.16	52,52,53,54	0
4	CO	B	612	1/1	0.93	0.07	67,67,67,67	0
3	SO4	B	601	5/5	0.93	0.20	52,52,53,54	0
3	SO4	D	603	5/5	0.93	0.11	28,29,31,32	0
3	SO4	D	604	5/5	0.93	0.21	38,41,43,43	0
4	CO	A	612	1/1	0.94	0.09	66,66,66,66	0
3	SO4	B	603	5/5	0.94	0.13	46,46,47,48	0
3	SO4	C	604	5/5	0.94	0.16	44,44,45,47	0
3	SO4	D	605	5/5	0.95	0.08	35,37,37,40	0
3	SO4	C	601	5/5	0.95	0.13	38,39,40,40	0
3	SO4	B	604	5/5	0.95	0.16	49,51,51,52	0
4	CO	C	613	1/1	0.95	0.09	95,95,95,95	0
4	CO	D	611	1/1	0.95	0.13	46,46,46,46	0
4	CO	D	612	1/1	0.95	0.09	66,66,66,66	0
4	CO	B	610	1/1	0.95	0.10	48,48,48,48	0
3	SO4	B	605	5/5	0.96	0.09	30,32,34,35	0
3	SO4	A	601	5/5	0.96	0.15	32,34,36,37	0
4	CO	C	610	1/1	0.97	0.07	47,47,47,47	0
4	CO	A	611	1/1	0.97	0.11	31,31,31,31	0
3	SO4	C	605	5/5	0.97	0.09	22,24,28,29	0
4	CO	D	610	1/1	0.99	0.10	35,35,35,35	0
4	CO	A	610	1/1	0.99	0.10	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.