Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:36 AM GMT

PDB ID	:	2XK1
Title	:	Crystal structure of a complex between Actinomadura R39 DD-peptidase and a boronate inhibitor
Authors	:	Sauvage, E.; Herman, R.; Kerff, F.; Rocaboy, M.; Charlier, P.
Deposited on	:	2010-07-07
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

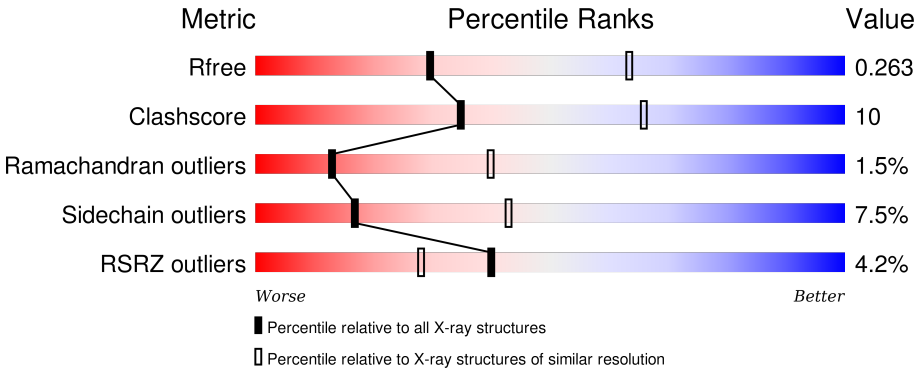
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 72% 26%
1	B	466	3% 77% 21%
1	C	466	3% 74% 23%
1	D	466	9% 80% 18%

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	EWB	B	500	-	-	-	X

2 Entry composition

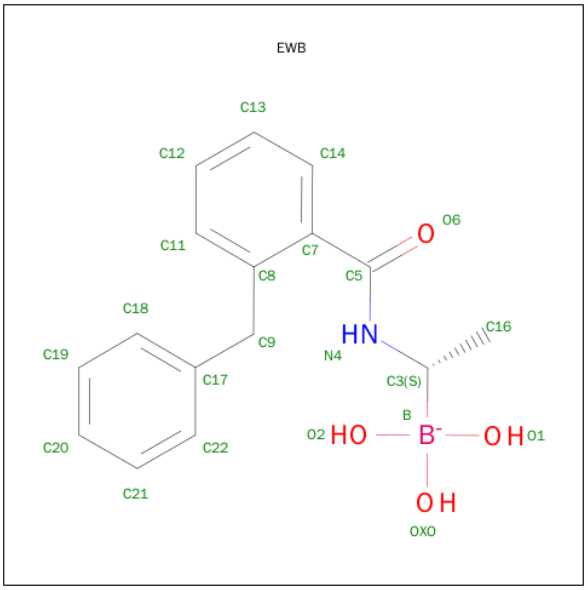
There are 5 unique types of molecules in this entry. The entry contains 13724 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			3352	2076	564	706	6			
1	B	465	Total	C	N	O	S	0	0	0
			3343	2071	563	703	6			
1	C	465	Total	C	N	O	S	0	0	0
			3343	2071	563	703	6			
1	D	466	Total	C	N	O	S	0	0	0
			3352	2076	564	706	6			

- Molecule 2 is [(1S)-1-{[(2-BENZYLPHENYL)CARBONYL]AMINO}ETHYL](TRIHYDROXY)BORATE(1-) (three-letter code: EWB) (formula: $C_{16}H_{19}BNO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	0	0
			21	1	16	1	3		
2	B	1	Total	B	C	N	O	0	0
			21	1	16	1	3		

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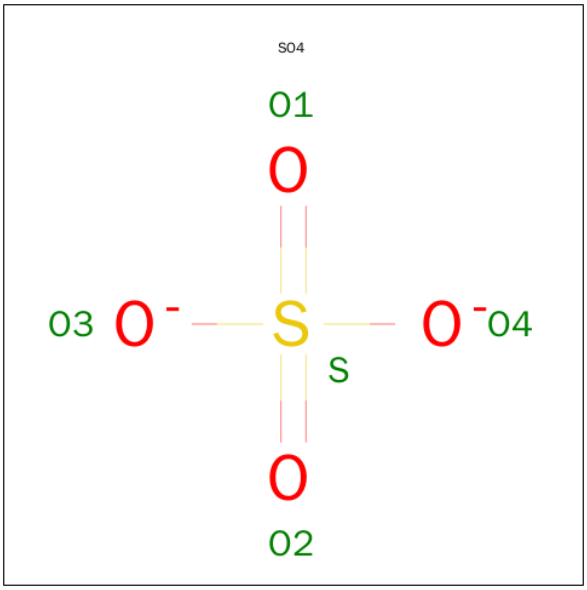
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total B C N O 21 1 16 1 3	0	0
2	D	1	Total B C N O 21 1 16 1 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: 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	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
3	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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

- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 5 is water.

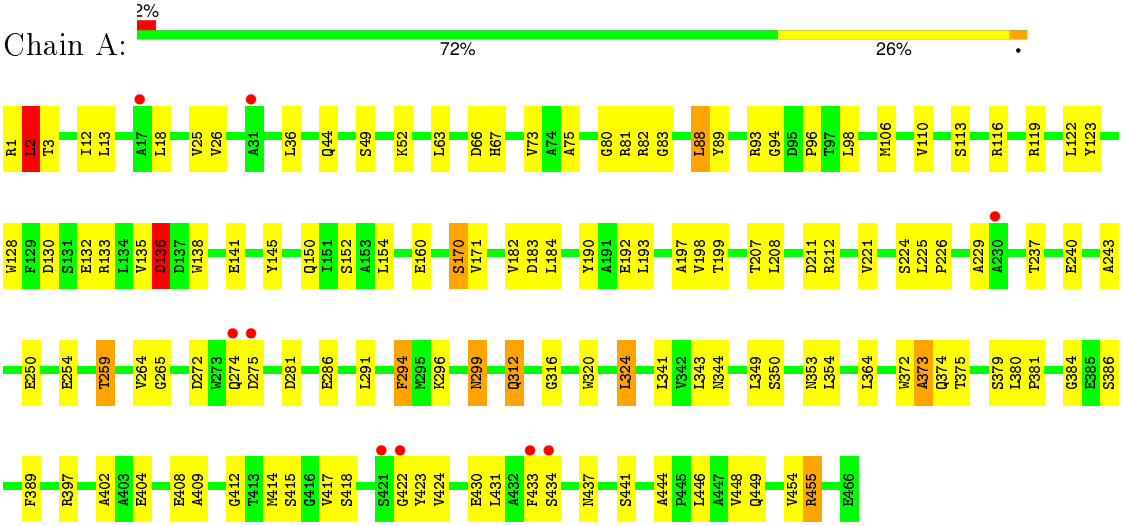
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	58	Total O 58 58	0	0
5	B	39	Total O 39 39	0	0
5	C	41	Total O 41 41	0	0
5	D	28	Total O 28 28	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

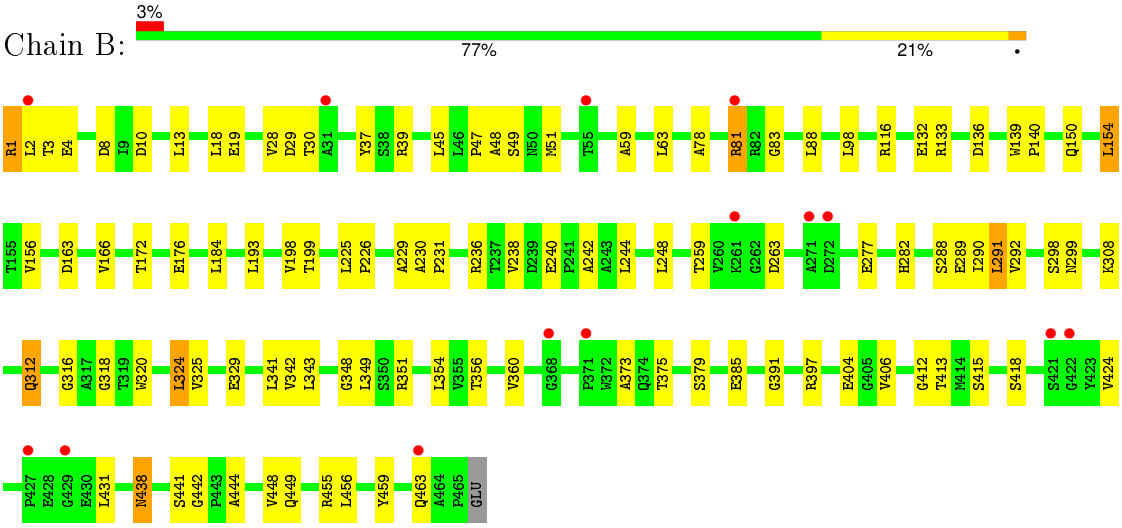
- Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain A:



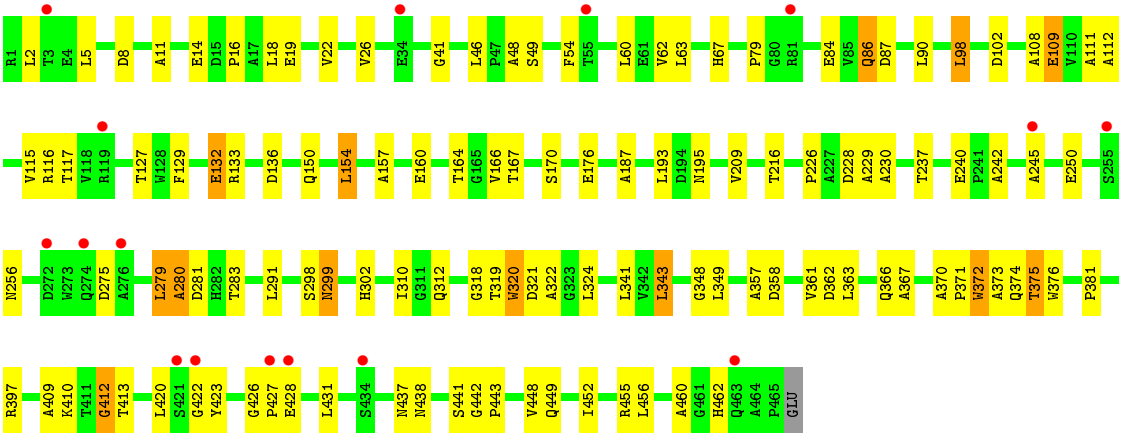
- Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain B:

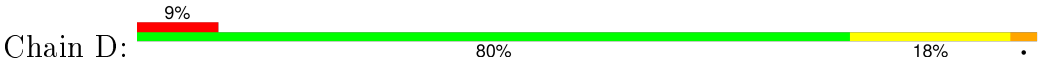


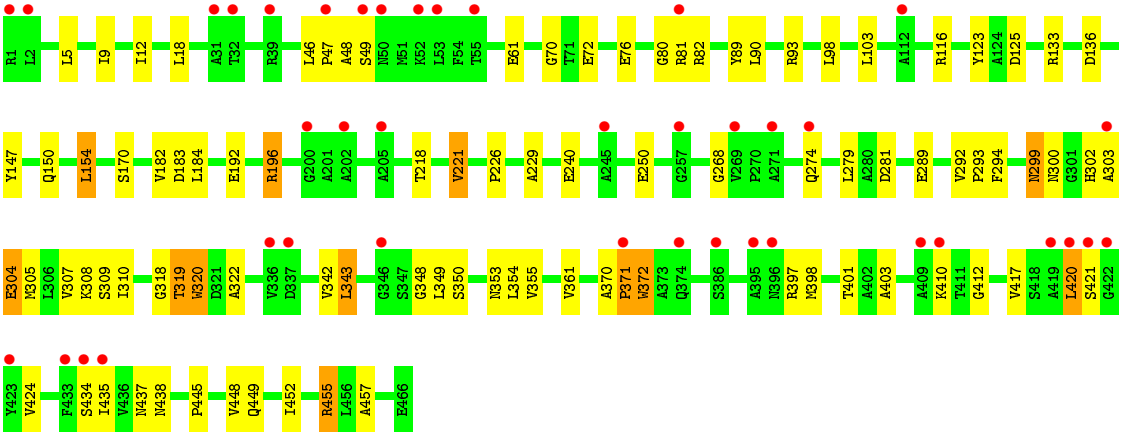
- Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain C:



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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.90Å 92.35Å 143.83Å 90.00° 92.25° 90.00°	Depositor
Resolution (Å)	27.53 – 2.80 27.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (27.53-2.80) 99.3 (27.53-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.264 0.216 , 0.263	Depositor DCC
R_{free} test set	2527 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	58.1	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.1	EDS
Estimated twinning fraction	0.000 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.000 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.004 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.015 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 49742 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13724	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: EWB, CO, 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	0.50	0/3411	0.67	0/4666
1	B	0.38	0/3402	0.58	0/4654
1	C	0.39	0/3402	0.57	0/4654
1	D	0.35	0/3411	0.53	0/4666
All	All	0.41	0/13626	0.59	0/18640

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	3352	0	3200	87	0
1	B	3343	0	3194	56	0
1	C	3343	0	3194	64	0
1	D	3352	0	3200	59	0
2	A	21	0	18	2	0
2	B	21	0	18	1	0
2	C	21	0	18	0	0
2	D	21	0	18	0	0
3	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	0	1	0
3	C	20	0	0	0	0
3	D	20	0	0	0	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	A	58	0	0	1	0
5	B	39	0	0	3	0
5	C	41	0	0	4	0
5	D	28	0	0	2	0
All	All	13724	0	12860	261	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 10.

All (261) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ASN:O	1:A:354:LEU:HD23	1.68	0.93
1:A:133:ARG:HB3	1:A:150:GLN:HG2	1.59	0.84
1:A:254:GLU:OE2	1:A:259:THR:HA	1.78	0.83
1:A:132:GLU:HG2	1:A:320:TRP:HZ3	1.47	0.79
1:A:226:PRO:HG2	1:A:229:ALA:HB2	1.69	0.74
1:A:397:ARG:HH12	1:A:449:GLN:HE21	1.35	0.74
2:A:500:EWB:H12	1:C:176:GLU:HB3	1.71	0.73
1:B:291:LEU:O	1:B:379:SER:HB2	1.88	0.73
1:B:83:GLY:HA3	1:B:116:ARG:NE	2.05	0.72
1:B:325:VAL:O	1:B:329:GLU:HG2	1.89	0.72
1:B:37:TYR:OH	1:B:39:ARG:HD2	1.90	0.71
1:A:408:GLU:O	1:A:422:GLY:HA3	1.92	0.69
1:D:182:VAL:HG21	1:D:221:VAL:HG21	1.74	0.69
1:B:83:GLY:HA3	1:B:116:ARG:HE	1.56	0.68
1:D:370:ALA:HB1	1:D:371:PRO:HD2	1.74	0.67
1:A:171:VAL:HG22	1:A:182:VAL:HG22	1.76	0.67
1:D:133:ARG:HB3	1:D:150:GLN:HB3	1.77	0.67
1:A:312:GLN:NE2	1:A:316:GLY:HA2	2.10	0.66
1:D:421:SER:HB3	1:D:434:SER:HA	1.76	0.66
1:C:48:ALA:O	1:C:348:GLY:HA3	1.96	0.66
1:A:136:ASP:HA	5:A:2020:HOH:O	1.96	0.65
1:D:72:GLU:HB3	1:D:281:ASP:HB3	1.77	0.65
1:A:93:ARG:HG2	1:A:128:TRP:CD2	2.31	0.65
1:A:150:GLN:HE22	1:A:240:GLU:H	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:LEU:HD21	1:D:445:PRO:HB3	1.80	0.64
1:C:370:ALA:HB1	1:C:371:PRO:HD2	1.79	0.64
1:C:133:ARG:HD2	1:C:150:GLN:HE21	1.63	0.63
1:D:170:SER:HB2	1:D:183:ASP:HB3	1.80	0.63
1:A:455:ARG:HA	1:A:455:ARG:HE	1.64	0.63
1:C:49:SER:HB2	1:C:412:GLY:HA2	1.79	0.63
1:C:426:GLY:HA2	1:C:462:HIS:NE2	2.14	0.62
1:A:225:LEU:HD12	1:A:226:PRO:HD2	1.81	0.62
1:A:52:LYS:HD3	1:A:294:PHE:CE2	2.34	0.62
1:C:341:LEU:HD13	1:C:343:LEU:HD21	1.81	0.62
1:A:397:ARG:HH12	1:A:449:GLN:NE2	1.98	0.62
1:D:292:VAL:HB	1:D:293:PRO:HD3	1.81	0.61
1:C:428:GLU:HA	5:C:2037:HOH:O	2.02	0.60
1:A:211:ASP:OD1	1:A:212:ARG:N	2.35	0.59
1:B:184:LEU:HD21	1:B:193:LEU:HD13	1.85	0.59
1:C:18:LEU:HD11	1:C:448:VAL:HG11	1.82	0.59
1:D:47:PRO:HB3	1:D:355:VAL:HG21	1.83	0.59
1:C:226:PRO:HG2	1:C:229:ALA:HB2	1.83	0.59
1:D:420:LEU:HD22	1:D:449:GLN:HB3	1.85	0.58
1:D:370:ALA:HB1	1:D:371:PRO:CD	2.34	0.58
1:A:132:GLU:HG2	1:A:320:TRP:CZ3	2.35	0.57
1:D:47:PRO:HB3	1:D:355:VAL:CG2	2.35	0.57
1:D:89:TYR:HE1	1:D:123:TYR:HD1	1.53	0.57
1:C:150:GLN:HE22	1:C:240:GLU:H	1.52	0.56
1:B:282:HIS:HA	3:B:601:SO4:O1	2.06	0.56
1:D:48:ALA:O	1:D:348:GLY:HA3	2.05	0.56
1:D:147:TYR:HB2	1:D:300:ASN:ND2	2.20	0.56
1:B:356:THR:O	1:B:360:VAL:HG23	2.05	0.56
1:B:1:ARG:HA	1:B:4:GLU:HB2	1.87	0.56
1:A:190:TYR:OH	1:A:243:ALA:HB3	2.05	0.56
1:D:303:ALA:O	1:D:307:VAL:HG23	2.06	0.55
1:A:133:ARG:NH2	1:A:152:SER:HB2	2.21	0.55
1:C:381:PRO:HG2	1:C:409:ALA:O	2.06	0.55
1:D:424:VAL:HG11	1:D:457:ALA:HA	1.87	0.55
1:D:9:ILE:HG23	1:D:452:ILE:HG12	1.89	0.54
1:A:381:PRO:HG2	1:A:409:ALA:O	2.07	0.54
1:A:192:GLU:HA	1:A:192:GLU:OE1	2.08	0.54
1:A:36:LEU:HD12	1:A:431:LEU:HD11	1.90	0.54
1:A:13:LEU:HD11	1:A:25:VAL:HG21	1.90	0.54
1:C:11:ALA:HA	1:C:14:GLU:HG2	1.90	0.54
1:C:16:PRO:O	1:C:19:GLU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:GLY:O	1:D:93:ARG:HB2	2.08	0.53
1:A:364:LEU:HD22	1:A:423:TYR:CE1	2.43	0.53
1:C:299:ASN:HD22	1:C:302:HIS:H	1.57	0.53
1:C:136:ASP:HA	5:C:2011:HOH:O	2.09	0.53
1:A:150:GLN:NE2	1:A:240:GLU:H	2.08	0.52
1:C:133:ARG:HD2	1:C:150:GLN:NE2	2.22	0.52
1:C:41:GLY:HA2	1:C:357:ALA:HB3	1.92	0.52
1:A:414:MET:HB2	1:A:417:VAL:HB	1.92	0.52
1:C:90:LEU:HG	1:C:154:LEU:HD11	1.91	0.52
2:A:500:EWB:C12	1:C:176:GLU:HB3	2.36	0.52
1:C:63:LEU:O	1:C:67:HIS:HB2	2.10	0.52
1:D:299:ASN:HD22	1:D:302:HIS:H	1.57	0.52
1:A:52:LYS:HD3	1:A:294:PHE:HE2	1.74	0.52
1:D:12:ILE:HG22	1:D:448:VAL:HG13	1.91	0.52
1:C:22:VAL:HG22	1:D:196:ARG:HG3	1.91	0.52
1:D:343:LEU:H	1:D:343:LEU:HD23	1.75	0.52
1:B:341:LEU:HD22	1:B:343:LEU:HG	1.92	0.51
1:C:111:ALA:HA	1:C:115:VAL:O	2.10	0.51
1:B:166:VAL:HA	1:B:236:ARG:O	2.11	0.51
1:A:49:SER:HB2	1:A:412:GLY:HA2	1.92	0.51
1:B:341:LEU:HD23	1:B:342:VAL:N	2.26	0.51
1:B:385:GLU:HB3	5:B:2035:HOH:O	2.10	0.51
1:A:455:ARG:HE	1:A:455:ARG:CA	2.23	0.51
1:A:296:LYS:HD3	1:A:379:SER:O	2.11	0.51
1:A:170:SER:HB2	1:A:183:ASP:HB2	1.91	0.51
1:D:90:LEU:HG	1:D:154:LEU:HD11	1.92	0.51
1:C:209:VAL:HG12	5:C:2030:HOH:O	2.09	0.50
1:A:207:THR:HA	1:C:230:ALA:HB1	1.92	0.50
1:C:132:GLU:HB3	1:C:320:TRP:HZ3	1.76	0.50
1:A:150:GLN:HE22	1:A:240:GLU:N	2.10	0.50
1:A:160:GLU:HG3	1:A:389:PHE:HZ	1.76	0.50
1:A:171:VAL:HG11	1:A:208:LEU:HD21	1.92	0.50
1:D:289:GLU:HG3	5:D:2017:HOH:O	2.10	0.50
1:A:63:LEU:O	1:A:67:HIS:HB2	2.11	0.50
1:C:150:GLN:NE2	1:C:240:GLU:H	2.09	0.49
1:A:312:GLN:HE21	1:A:316:GLY:HA2	1.76	0.49
1:A:184:LEU:HD11	1:A:193:LEU:HB2	1.94	0.49
1:A:198:VAL:HG11	1:B:19:GLU:HG3	1.93	0.49
1:B:1:ARG:HE	1:B:1:ARG:N	2.10	0.49
1:D:89:TYR:CE1	1:D:123:TYR:HD1	2.29	0.49
1:A:372:TRP:O	1:A:374:GLN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLN:HB3	1:A:354:LEU:HD13	1.94	0.49
1:B:320:TRP:O	1:B:324:LEU:HB2	2.12	0.49
1:B:424:VAL:HB	1:B:431:LEU:HB2	1.95	0.49
1:A:75:ALA:HB2	1:A:88:LEU:HD23	1.93	0.49
1:D:46:LEU:HB2	1:D:417:VAL:HG21	1.94	0.49
1:D:294:PHE:HE2	1:D:303:ALA:HB2	1.78	0.48
1:A:66:ASP:O	1:A:286:GLU:HG2	2.12	0.48
1:C:397:ARG:HH12	1:C:449:GLN:HE21	1.60	0.48
1:A:160:GLU:HG3	1:A:389:PHE:CZ	2.48	0.48
1:A:198:VAL:O	1:A:224:SER:HA	2.14	0.48
1:B:198:VAL:HG22	1:B:199:THR:H	1.78	0.48
1:D:61:GLU:HG2	1:D:372:TRP:HZ2	1.78	0.48
1:D:226:PRO:HG2	1:D:229:ALA:HB2	1.95	0.48
1:A:106:MET:O	1:A:110:VAL:HG23	2.13	0.48
1:A:80:GLY:O	1:A:83:GLY:N	2.42	0.48
1:C:423:TYR:HA	1:C:431:LEU:O	2.13	0.48
1:D:184:LEU:H	1:D:184:LEU:HD12	1.78	0.48
1:B:238:VAL:HG21	1:B:244:LEU:HD22	1.95	0.48
1:A:294:PHE:C	1:A:294:PHE:CD2	2.85	0.47
1:A:49:SER:O	1:A:52:LYS:HB2	2.14	0.47
1:D:437:ASN:C	1:D:438:ASN:HD22	2.17	0.47
1:B:397:ARG:HH12	1:B:449:GLN:HE21	1.61	0.47
1:C:427:PRO:HD3	1:C:462:HIS:NE2	2.29	0.47
1:B:51:MET:SD	1:B:343:LEU:HD23	2.54	0.47
1:B:308:LYS:HG2	1:B:318:GLY:C	2.34	0.47
1:A:49:SER:OG	1:A:52:LYS:NZ	2.46	0.47
1:B:48:ALA:O	1:B:348:GLY:HA3	2.14	0.47
1:C:166:VAL:HG12	1:C:237:THR:HA	1.96	0.47
1:A:384:GLY:HA3	1:A:404:GLU:HG3	1.97	0.47
1:D:49:SER:HB2	1:D:412:GLY:HA2	1.96	0.47
1:C:84:GLU:HG2	1:C:117:THR:HB	1.95	0.47
1:D:397:ARG:HH12	1:D:449:GLN:HE21	1.61	0.47
1:B:226:PRO:HG2	1:B:229:ALA:HB2	1.96	0.47
1:A:444:ALA:O	1:A:446:LEU:N	2.46	0.47
1:B:47:PRO:HD2	5:B:2034:HOH:O	2.13	0.47
1:A:135:VAL:O	1:A:136:ASP:C	2.52	0.47
1:C:193:LEU:HD11	1:C:195:ASN:HB2	1.97	0.46
1:A:133:ARG:HB3	1:A:150:GLN:CG	2.39	0.46
1:A:299:ASN:C	1:A:299:ASN:HD22	2.19	0.46
1:D:305:MET:O	1:D:309:SER:OG	2.30	0.46
1:A:372:TRP:O	1:A:373:ALA:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:ARG:HB2	1:B:459:TYR:CE1	2.51	0.46
1:B:263:ASP:HB3	5:B:2030:HOH:O	2.15	0.46
1:C:319:THR:HG22	1:C:322:ALA:H	1.80	0.46
1:B:156:VAL:HG21	1:B:248:LEU:HD13	1.97	0.46
1:B:28:VAL:HG12	1:B:29:ASP:N	2.30	0.46
1:D:319:THR:HG22	1:D:322:ALA:HB3	1.98	0.46
1:A:135:VAL:HB	1:A:138:TRP:CD1	2.51	0.46
1:B:18:LEU:HD12	1:B:448:VAL:HG11	1.97	0.46
1:A:312:GLN:HE21	1:A:312:GLN:CA	2.28	0.46
1:C:108:ALA:HB2	1:C:256:ASN:OD1	2.16	0.46
1:A:324:LEU:HD12	1:A:324:LEU:HA	1.79	0.46
1:B:230:ALA:HB1	1:B:231:PRO:HD2	1.97	0.46
1:C:109:GLU:HA	1:C:112:ALA:HB3	1.98	0.45
1:C:397:ARG:HH12	1:C:449:GLN:NE2	2.14	0.45
1:A:12:ILE:HG22	1:A:448:VAL:HG13	1.99	0.45
1:B:59:ALA:O	1:B:63:LEU:HB2	2.16	0.45
1:C:26:VAL:CG1	1:C:361:VAL:HG21	2.46	0.45
1:C:362:ASP:O	1:C:366:GLN:HG2	2.16	0.45
1:D:5:LEU:HD12	1:D:455:ARG:NE	2.32	0.45
1:A:197:ALA:HB2	1:A:221:VAL:HG12	1.99	0.45
1:A:150:GLN:NE2	1:A:240:GLU:N	2.65	0.45
1:A:412:GLY:O	1:A:418:SER:HA	2.17	0.45
1:D:319:THR:HG23	1:D:322:ALA:H	1.82	0.45
1:D:370:ALA:HB3	5:D:2020:HOH:O	2.17	0.44
1:B:163:ASP:O	1:B:166:VAL:HG22	2.17	0.44
1:C:452:ILE:O	1:C:456:LEU:HG	2.17	0.44
1:C:426:GLY:HA3	1:C:460:ALA:HB1	2.00	0.44
1:A:2:LEU:HD21	1:A:36:LEU:HD22	1.98	0.44
1:A:123:TYR:HA	1:A:265:GLY:O	2.18	0.44
1:C:167:THR:HG21	1:C:187:ALA:HB3	1.98	0.44
1:C:154:LEU:HD22	1:C:245:ALA:CB	2.47	0.44
1:D:61:GLU:HG2	1:D:372:TRP:CZ2	2.52	0.44
1:D:89:TYR:HD1	1:D:123:TYR:HB2	1.82	0.44
1:D:9:ILE:HA	1:D:12:ILE:HD12	2.00	0.44
1:C:26:VAL:HG12	1:C:361:VAL:HG21	2.00	0.44
1:A:199:THR:HA	1:A:225:LEU:O	2.17	0.44
1:D:437:ASN:ND2	1:D:445:PRO:HG2	2.33	0.44
1:C:129:PHE:HA	1:C:318:GLY:HA3	2.00	0.44
1:D:89:TYR:CD1	1:D:123:TYR:HB2	2.52	0.44
1:D:196:ARG:HB3	1:D:196:ARG:HH11	1.82	0.44
1:B:225:LEU:HD12	1:B:226:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LEU:HD11	1:C:291:LEU:HD11	1.99	0.44
1:A:341:LEU:HD13	1:A:343:LEU:HD21	2.00	0.44
1:D:410:LYS:O	1:D:420:LEU:HA	2.18	0.44
1:D:307:VAL:HA	1:D:310:ILE:HD12	2.00	0.43
1:C:372:TRP:O	1:C:374:GLN:N	2.51	0.43
1:C:157:ALA:HA	1:C:164:THR:HA	2.00	0.43
1:C:115:VAL:HG12	1:C:116:ARG:N	2.33	0.43
1:B:18:LEU:CD1	1:B:448:VAL:HG11	2.49	0.43
1:B:81:ARG:H	1:B:81:ARG:HG2	1.62	0.43
1:B:133:ARG:HB3	1:B:150:GLN:HB3	2.00	0.43
1:B:150:GLN:NE2	1:B:240:GLU:H	2.17	0.43
1:B:341:LEU:CD2	1:B:343:LEU:HG	2.48	0.43
1:C:132:GLU:HB3	1:C:320:TRP:CZ3	2.53	0.43
1:B:412:GLY:O	1:B:418:SER:HA	2.19	0.43
1:D:308:LYS:O	1:D:318:GLY:HA2	2.19	0.43
1:A:424:VAL:HB	1:A:431:LEU:HB3	2.00	0.43
1:A:312:GLN:HE21	1:A:312:GLN:HA	1.84	0.43
1:C:279:LEU:O	1:C:280:ALA:HB2	2.19	0.43
1:B:13:LEU:HD12	1:B:39:ARG:HH11	1.82	0.43
1:D:420:LEU:HD23	1:D:435:ILE:HD12	2.01	0.43
1:A:145:TYR:O	1:A:237:THR:HG23	2.19	0.42
1:A:25:VAL:HA	1:A:434:SER:O	2.20	0.42
1:D:343:LEU:HD23	1:D:343:LEU:N	2.33	0.42
1:B:78:ALA:HA	1:B:277:GLU:HG2	2.01	0.42
1:D:398:MET:O	1:D:401:THR:OG1	2.36	0.42
1:B:342:VAL:HB	1:B:354:LEU:HB2	2.00	0.42
1:B:154:LEU:O	1:B:242:ALA:HA	2.18	0.42
1:A:26:VAL:O	1:A:433:PHE:HA	2.20	0.42
1:C:86:GLN:HB3	1:C:87:ASP:H	1.57	0.42
1:D:196:ARG:NH1	1:D:196:ARG:HB3	2.35	0.42
1:A:80:GLY:O	1:A:82:ARG:N	2.53	0.42
1:A:18:LEU:HD11	1:A:448:VAL:HG11	2.02	0.42
1:A:73:VAL:HA	1:A:89:TYR:O	2.19	0.42
1:C:367:ALA:HB3	1:C:423:TYR:OH	2.20	0.42
1:A:130:ASP:OD1	1:A:130:ASP:C	2.58	0.42
1:B:397:ARG:HH12	1:B:449:GLN:NE2	2.18	0.42
1:C:54:PHE:CD2	1:C:363:LEU:HD22	2.55	0.42
1:C:299:ASN:ND2	1:C:302:HIS:H	2.16	0.42
1:C:298:SER:HB2	1:C:410:LYS:NZ	2.35	0.42
1:D:350:SER:HB3	1:D:353:ASN:ND2	2.35	0.41
1:D:125:ASP:OD1	1:D:268:GLY:HA2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:GLU:HA	1:A:240:GLU:OE1	2.20	0.41
1:A:437:ASN:ND2	1:A:449:GLN:OE1	2.53	0.41
1:D:304:GLU:HG3	1:D:320:TRP:HZ2	1.84	0.41
1:C:409:ALA:HA	1:C:422:GLY:HA3	2.02	0.41
1:A:372:TRP:O	1:A:375:THR:HG22	2.20	0.41
1:A:93:ARG:HG2	1:A:128:TRP:CE3	2.55	0.41
1:C:98:LEU:HD23	1:C:102:ASP:HB2	2.03	0.41
1:C:62:VAL:HG11	1:C:310:ILE:HG23	2.01	0.41
1:A:344:ASN:ND2	1:A:350:SER:OG	2.44	0.41
1:D:401:THR:C	1:D:403:ALA:H	2.22	0.41
1:B:290:ILE:C	1:B:292:VAL:H	2.23	0.41
1:B:404:GLU:O	1:B:406:VAL:HG23	2.21	0.41
1:A:402:ALA:HB3	1:A:454:VAL:HG13	2.03	0.41
1:A:94:GLY:O	1:A:96:PRO:HD3	2.21	0.41
1:C:242:ALA:O	1:C:245:ALA:HB3	2.21	0.41
1:B:288:SER:HB2	1:B:375:THR:OG1	2.21	0.41
1:B:312:GLN:NE2	1:B:316:GLY:HA2	2.36	0.41
1:D:342:VAL:HB	1:D:354:LEU:HB2	2.03	0.41
1:B:139:TRP:HA	1:B:140:PRO:HD2	1.90	0.41
1:A:122:LEU:HD23	1:A:264:VAL:HG22	2.02	0.41
1:B:385:GLU:HB2	1:B:391:GLY:CA	2.51	0.41
1:A:145:TYR:OH	1:C:228:ASP:HB3	2.20	0.41
1:C:443:PRO:HB2	5:C:2039:HOH:O	2.20	0.41
1:D:192:GLU:HB2	1:D:218:THR:HA	2.03	0.41
1:C:420:LEU:HB2	1:C:449:GLN:NE2	2.36	0.40
1:B:28:VAL:CG1	1:B:29:ASP:N	2.84	0.40
1:D:47:PRO:HG3	1:D:355:VAL:HG13	2.03	0.40
1:B:45:LEU:HD22	1:B:438:ASN:HB2	2.03	0.40
1:A:207:THR:HG21	1:B:441:SER:OG	2.22	0.40
1:C:375:THR:OG1	1:C:375:THR:O	2.35	0.40
1:B:424:VAL:HG21	1:B:456:LEU:HB3	2.04	0.40
1:B:49:SER:CB	2:B:500:EWB:O1	2.70	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%)	416 (90%)	43 (9%)	5 (1%)	17 50
1	B	463/466 (99%)	422 (91%)	34 (7%)	7 (2%)	13 40
1	C	463/466 (99%)	425 (92%)	28 (6%)	10 (2%)	8 28
1	D	464/466 (100%)	421 (91%)	37 (8%)	6 (1%)	15 44
All	All	1854/1864 (100%)	1684 (91%)	142 (8%)	28 (2%)	13 40

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	A	373	ALA
1	C	79	PRO
1	C	373	ALA
1	A	136	ASP
1	A	415	SER
1	C	86	GLN
1	C	280	ALA
1	A	2	LEU
1	B	176	GLU
1	B	373	ALA
1	B	415	SER
1	C	127	THR
1	D	80	GLY
1	B	98	LEU
1	B	291	LEU
1	C	2	LEU
1	C	109	GLU
1	D	76	GLU
1	D	371	PRO
1	D	372	TRP
1	B	442	GLY
1	B	444	ALA
1	C	441	SER
1	D	279	LEU
1	D	240	GLU
1	C	442	GLY
1	C	412	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	339/339 (100%)	310 (91%)	29 (9%)	13	36
1	B	338/339 (100%)	314 (93%)	24 (7%)	18	46
1	C	338/339 (100%)	309 (91%)	29 (9%)	13	36
1	D	339/339 (100%)	319 (94%)	20 (6%)	24	57
All	All	1354/1356 (100%)	1252 (92%)	102 (8%)	17	43

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	A	2	LEU
1	A	3	THR
1	A	88	LEU
1	A	98	LEU
1	A	113	SER
1	A	116	ARG
1	A	119	ARG
1	A	136	ASP
1	A	141	GLU
1	A	154	LEU
1	A	170	SER
1	A	250	GLU
1	A	259	THR
1	A	272	ASP
1	A	274	GLN
1	A	275	ASP
1	A	281	ASP
1	A	291	LEU
1	A	294	PHE
1	A	299	ASN
1	A	312	GLN
1	A	324	LEU
1	A	349	LEU

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Mol	Chain	Res	Type
1	A	380	LEU
1	A	386	SER
1	A	430	GLU
1	A	441	SER
1	A	455	ARG
1	B	1	ARG
1	B	2	LEU
1	B	3	THR
1	B	8	ASP
1	B	10	ASP
1	B	30	THR
1	B	81	ARG
1	B	88	LEU
1	B	132	GLU
1	B	136	ASP
1	B	154	LEU
1	B	172	THR
1	B	259	THR
1	B	289	GLU
1	B	298	SER
1	B	299	ASN
1	B	312	GLN
1	B	324	LEU
1	B	349	LEU
1	B	351	ARG
1	B	413	THR
1	B	438	ASN
1	B	455	ARG
1	B	463	GLN
1	C	5	LEU
1	C	8	ASP
1	C	46	LEU
1	C	98	LEU
1	C	132	GLU
1	C	154	LEU
1	C	160	GLU
1	C	170	SER
1	C	216	THR
1	C	250	GLU
1	C	275	ASP
1	C	279	LEU
1	C	281	ASP

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Mol	Chain	Res	Type
1	C	283	THR
1	C	299	ASN
1	C	312	GLN
1	C	320	TRP
1	C	321	ASP
1	C	324	LEU
1	C	343	LEU
1	C	349	LEU
1	C	358	ASP
1	C	372	TRP
1	C	375	THR
1	C	376	TRP
1	C	413	THR
1	C	437	ASN
1	C	438	ASN
1	C	455	ARG
1	D	81	ARG
1	D	82	ARG
1	D	98	LEU
1	D	103	LEU
1	D	116	ARG
1	D	136	ASP
1	D	154	LEU
1	D	196	ARG
1	D	221	VAL
1	D	250	GLU
1	D	274	GLN
1	D	299	ASN
1	D	304	GLU
1	D	319	THR
1	D	320	TRP
1	D	343	LEU
1	D	349	LEU
1	D	361	VAL
1	D	420	LEU
1	D	455	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	150	GLN

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Mol	Chain	Res	Type
1	A	158	HIS
1	A	299	ASN
1	A	312	GLN
1	A	437	ASN
1	A	438	ASN
1	A	449	GLN
1	B	44	GLN
1	B	150	GLN
1	B	299	ASN
1	B	312	GLN
1	B	366	GLN
1	B	437	ASN
1	B	449	GLN
1	B	463	GLN
1	C	150	GLN
1	C	299	ASN
1	C	312	GLN
1	C	366	GLN
1	C	437	ASN
1	C	449	GLN
1	D	50	ASN
1	D	150	GLN
1	D	274	GLN
1	D	299	ASN
1	D	312	GLN
1	D	437	ASN
1	D	449	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EWB	A	500	1	21,22,23	0.68	0	22,29,32	0.76	0
3	SO4	A	601	-	4,4,4	0.17	0	6,6,6	0.31	0
3	SO4	A	602	-	4,4,4	0.12	0	6,6,6	0.10	0
3	SO4	A	603	-	4,4,4	0.11	0	6,6,6	0.73	0
3	SO4	A	604	-	4,4,4	0.18	0	6,6,6	0.12	0
2	EWB	B	500	1	21,22,23	0.73	0	22,29,32	0.70	0
3	SO4	B	601	-	4,4,4	0.08	0	6,6,6	0.44	0
3	SO4	B	602	-	4,4,4	0.14	0	6,6,6	0.12	0
3	SO4	B	603	-	4,4,4	0.09	0	6,6,6	0.17	0
3	SO4	B	604	-	4,4,4	0.17	0	6,6,6	0.08	0
2	EWB	C	500	1	21,22,23	0.65	0	22,29,32	0.62	0
3	SO4	C	601	-	4,4,4	0.14	0	6,6,6	0.29	0
3	SO4	C	602	-	4,4,4	0.11	0	6,6,6	0.21	0
3	SO4	C	603	-	4,4,4	0.16	0	6,6,6	0.26	0
3	SO4	C	604	-	4,4,4	0.15	0	6,6,6	0.22	0
2	EWB	D	500	1	21,22,23	0.71	0	22,29,32	0.79	0
3	SO4	D	601	-	4,4,4	0.17	0	6,6,6	0.15	0
3	SO4	D	602	-	4,4,4	0.10	0	6,6,6	0.09	0
3	SO4	D	603	-	4,4,4	0.20	0	6,6,6	0.09	0
3	SO4	D	604	-	4,4,4	0.13	0	6,6,6	0.09	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	EWB	A	500	1	-	0/11/16/18	0/2/2/2
3	SO4	A	601	-	-	0/0/0/0	0/0/0/0
3	SO4	A	602	-	-	0/0/0/0	0/0/0/0
3	SO4	A	603	-	-	0/0/0/0	0/0/0/0
3	SO4	A	604	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EWB	B	500	1	-	0/11/16/18	0/2/2/2
3	SO4	B	601	-	-	0/0/0/0	0/0/0/0
3	SO4	B	602	-	-	0/0/0/0	0/0/0/0
3	SO4	B	603	-	-	0/0/0/0	0/0/0/0
3	SO4	B	604	-	-	0/0/0/0	0/0/0/0
2	EWB	C	500	1	-	0/11/16/18	0/2/2/2
3	SO4	C	601	-	-	0/0/0/0	0/0/0/0
3	SO4	C	602	-	-	0/0/0/0	0/0/0/0
3	SO4	C	603	-	-	0/0/0/0	0/0/0/0
3	SO4	C	604	-	-	0/0/0/0	0/0/0/0
2	EWB	D	500	1	-	0/11/16/18	0/2/2/2
3	SO4	D	601	-	-	0/0/0/0	0/0/0/0
3	SO4	D	602	-	-	0/0/0/0	0/0/0/0
3	SO4	D	603	-	-	0/0/0/0	0/0/0/0
3	SO4	D	604	-	-	0/0/0/0	0/0/0/0

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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	EWB	2	0
2	B	500	EWB	1	0
3	B	601	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	466/466 (100%)	-0.26	9 (1%) 70 59	13, 45, 82, 107	0
1	B	465/466 (99%)	-0.03	14 (3%) 54 41	39, 66, 97, 118	0
1	C	465/466 (99%)	0.07	16 (3%) 49 36	32, 71, 109, 144	0
1	D	466/466 (100%)	0.37	40 (8%) 13 6	69, 87, 118, 140	0
All	All	1862/1864 (99%)	0.04	79 (4%) 40 28	13, 70, 108, 144	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	421	SER	5.0
1	D	422	GLY	4.9
1	D	421	SER	4.6
1	D	31	ALA	4.4
1	D	274	GLN	4.2
1	C	272	ASP	4.1
1	A	31	ALA	3.9
1	C	422	GLY	3.4
1	D	2	LEU	3.3
1	D	81	ARG	3.2
1	B	422	GLY	3.1
1	D	396	ASN	3.1
1	B	2	LEU	3.1
1	D	410	LYS	3.1
1	D	55	THR	2.9
1	B	427	PRO	2.9
1	D	336	VAL	2.9
1	C	274	GLN	2.8
1	D	386	SER	2.8
1	C	3	THR	2.7
1	A	433	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	337	ASP	2.7
1	D	245	ALA	2.7
1	C	55	THR	2.7
1	B	31	ALA	2.6
1	D	371	PRO	2.6
1	A	422	GLY	2.6
1	B	271	ALA	2.6
1	C	427	PRO	2.5
1	A	275	ASP	2.5
1	B	272	ASP	2.5
1	D	50	ASN	2.5
1	C	434	SER	2.5
1	B	81	ARG	2.5
1	D	49	SER	2.5
1	D	271	ALA	2.5
1	C	276	ALA	2.4
1	D	419	ALA	2.4
1	D	32	THR	2.4
1	D	409	ALA	2.4
1	B	429	GLY	2.4
1	D	303	ALA	2.3
1	D	433	PHE	2.3
1	A	17	ALA	2.3
1	D	1	ARG	2.3
1	D	52	LYS	2.3
1	C	81	ARG	2.3
1	C	463	GLN	2.3
1	D	200	GLY	2.3
1	D	205	ALA	2.2
1	D	53	LEU	2.2
1	D	420	LEU	2.2
1	C	428	GLU	2.2
1	A	421	SER	2.2
1	D	374	GLN	2.2
1	A	434	SER	2.2
1	D	257	GLY	2.2
1	D	202	ALA	2.2
1	B	371	PRO	2.2
1	D	395	ALA	2.2
1	D	47	PRO	2.1
1	D	346	GLY	2.1
1	A	274	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	255	SER	2.1
1	B	261	LYS	2.1
1	D	434	SER	2.1
1	D	39	ARG	2.1
1	B	55	THR	2.1
1	C	245	ALA	2.1
1	B	463	GLN	2.1
1	B	368	GLY	2.1
1	B	421	SER	2.1
1	C	34	GLU	2.0
1	D	435	ILE	2.0
1	D	423	TYR	2.0
1	A	230	ALA	2.0
1	C	119	ARG	2.0
1	D	269	VAL	2.0
1	D	112	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	EWB	B	500	21/22	0.91	0.34	2.72	50,56,61,62	0
2	EWB	C	500	21/22	0.89	0.34	1.49	62,64,66,66	0
2	EWB	D	500	21/22	0.83	0.32	1.03	67,70,73,73	0
3	SO4	C	604	5/5	0.89	0.20	0.78	93,93,94,94	0
3	SO4	D	604	5/5	0.76	0.32	0.53	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	EWB	A	500	21/22	0.94	0.19	-0.33	30,39,40,41	0
4	CO	A	610	1/1	0.98	0.06	-1.56	58,58,58,58	0
4	CO	D	610	1/1	0.93	0.07	-1.68	95,95,95,95	0
4	CO	D	611	1/1	0.87	0.10	-2.09	110,110,110,110	0
4	CO	A	611	1/1	0.97	0.04	-2.66	48,48,48,48	0
3	SO4	D	603	5/5	0.80	0.25	-	133,133,134,134	0
3	SO4	B	603	5/5	0.98	0.13	-	53,54,54,55	0
3	SO4	B	604	5/5	0.85	0.23	-	135,135,135,135	0
3	SO4	D	602	5/5	0.92	0.13	-	106,106,106,106	0
3	SO4	C	602	5/5	0.97	0.17	-	55,55,55,56	0
3	SO4	C	601	5/5	0.93	0.18	-	60,60,62,63	0
3	SO4	A	604	5/5	0.93	0.24	-	88,88,88,88	0
3	SO4	D	601	5/5	0.82	0.26	-	107,107,108,108	0
3	SO4	A	603	5/5	0.99	0.17	-	40,40,41,41	0
3	SO4	B	602	5/5	0.98	0.14	-	71,71,71,72	0
3	SO4	B	601	5/5	0.90	0.32	-	64,64,65,66	0
3	SO4	A	602	5/5	0.95	0.16	-	78,78,79,79	0
3	SO4	A	601	5/5	0.96	0.10	-	60,60,61,62	0
3	SO4	C	603	5/5	0.96	0.18	-	62,62,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.