W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:32 AM GMT

PDB ID : 3IT9
Title : Crystal structure of Penicillin-Binding Protein 6 (PBP6) from E. coli in apo state
Authors : Chen, Y.; Zhang, W.; Shi, Q.; Hesek, D.; Lee, M.; Mobashery, S.; Shoichet, B.K.
Deposited on : 2009-08-27
Resolution : 2.10 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 (i)) 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 2.10 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.
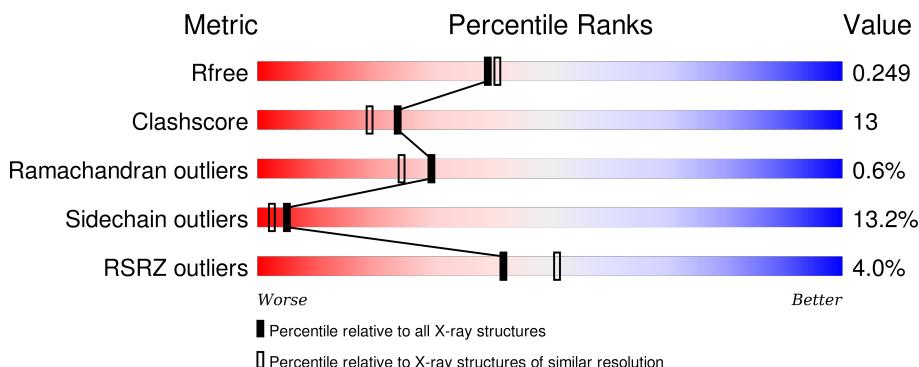
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	352	
1	B	352	
1	C	352	
1	D	352	
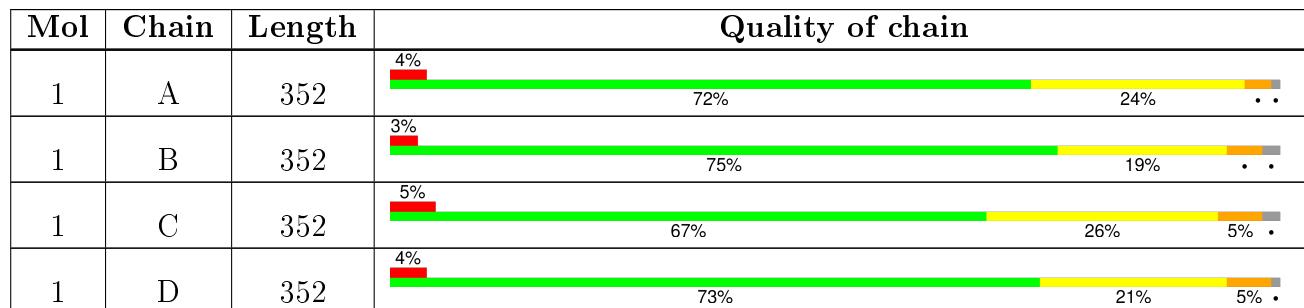
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	D	354	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11144 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 dacC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total 2674	C 1687	N 465	O 512	S 10	0	3	0
1	B	345	Total 2649	C 1675	N 455	O 509	S 10	0	3	0
1	C	345	Total 2638	C 1667	N 454	O 506	S 11	0	2	0
1	D	350	Total 2676	C 1690	N 461	O 515	S 10	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P08506
B	1	MET	-	INITIATING METHIONINE	UNP P08506
C	1	MET	-	INITIATING METHIONINE	UNP P08506
D	1	MET	-	INITIATING METHIONINE	UNP P08506

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
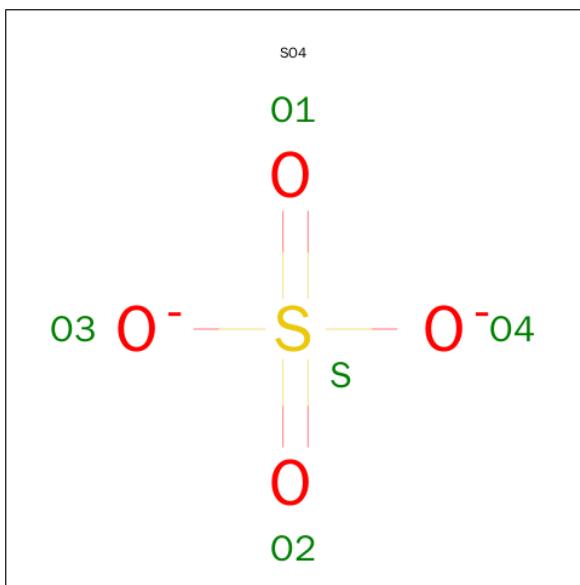
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0

- Molecule 3 is sucrose (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).
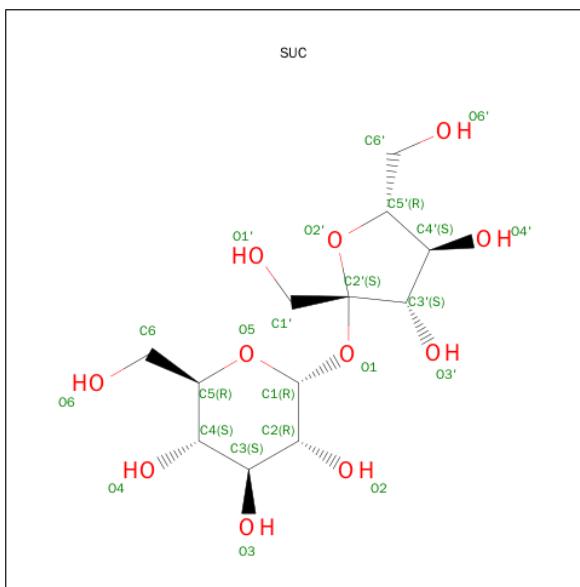
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 23	C 12	O 11	0	0
3	A	1	Total 23	C 12	O 11	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	126	Total 126	O 126	0	0
4	B	107	Total 107	O 107	0	0
4	C	87	Total 87	O 87	0	0
4	D	101	Total 101	O 101	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 dacC
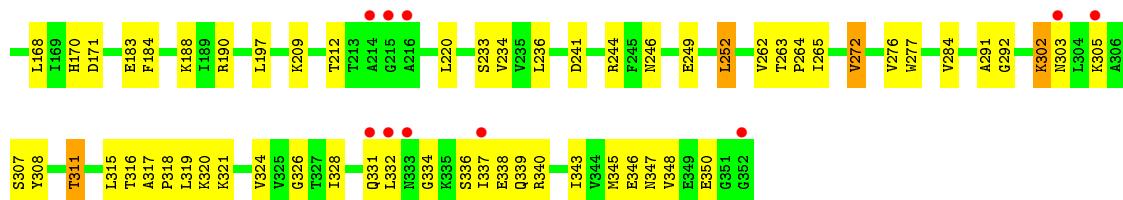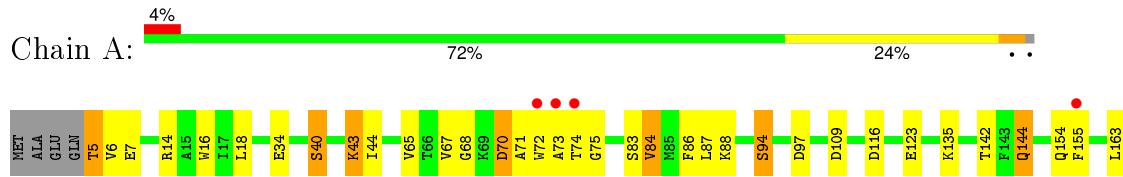
- Molecule 1: D-alanyl-D-alanine carboxypeptidase dacC

- Molecule 1: D-alanyl-D-alanine carboxypeptidase dacC

• Molecule 1: D-alanyl-D-alanine carboxypeptidase dacC

Chain D:
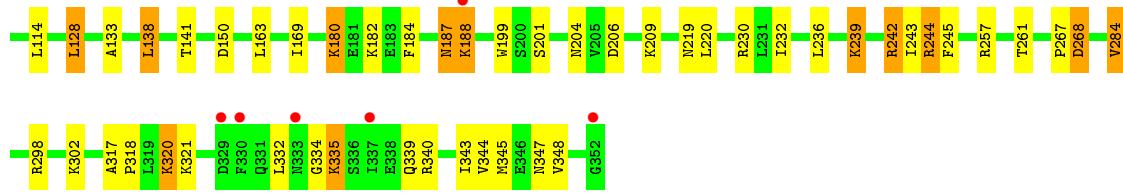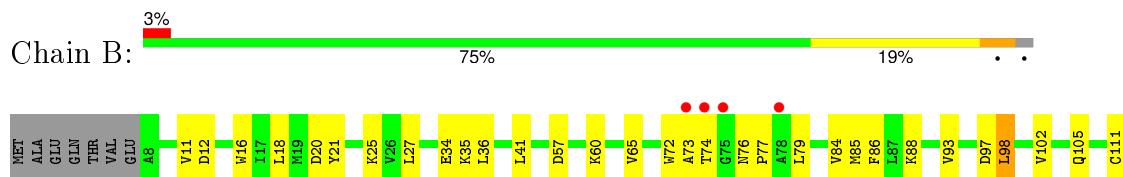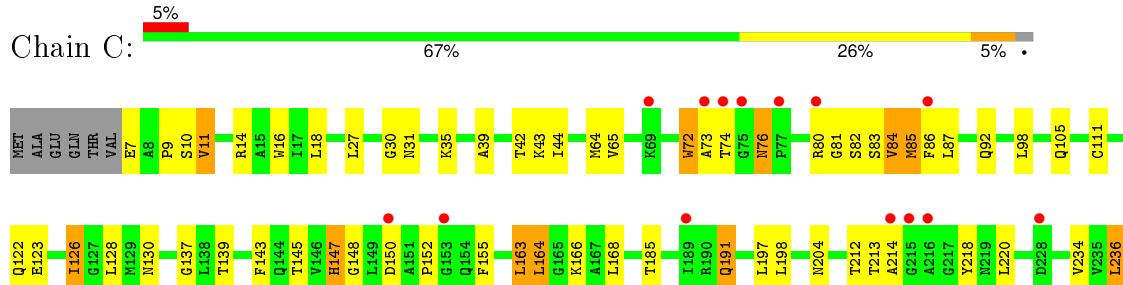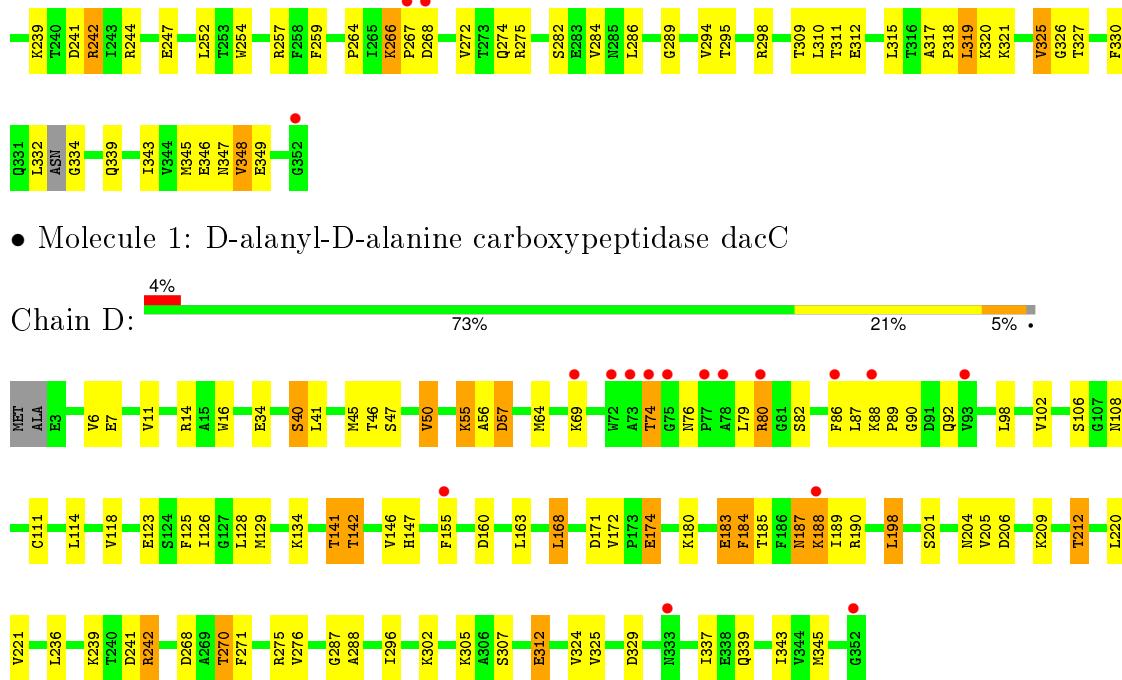
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.95Å 184.85Å 81.61Å 90.00° 100.62° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 48.86 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-2.10) 97.2 (48.86-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.207 , 0.259 0.201 , 0.249	Depositor DCC
R_{free} test set	4673 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.631	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 93444 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11144	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SUC, 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	0.61	0/2722	0.49	0/3682
1	B	0.56	1/2695 (0.0%)	0.47	0/3645
1	C	0.52	0/2685	0.46	0/3629
1	D	0.56	0/2727	0.45	0/3688
All	All	0.56	1/10829 (0.0%)	0.47	0/14644

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	CYS	CB-SG	-5.23	1.73	1.81

There are no bond angle outliers.

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	2674	0	2706	64	0
1	B	2649	0	2670	70	0
1	C	2638	0	2667	77	0
1	D	2676	0	2709	78	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	1	0
2	D	15	0	0	4	0
3	A	46	0	44	1	0
4	A	126	0	0	0	0
4	B	107	0	0	3	0
4	C	87	0	0	2	0
4	D	101	0	0	10	0
All	All	11144	0	10796	283	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 13.

All (283) 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:343:ILE:HG13	1:A:345:MET:CE	1.64	1.26
1:B:334:GLY:CA	1:B:335:LYS:HB2	1.63	1.24
1:B:334:GLY:HA3	1:B:335:LYS:CB	1.63	1.22
1:B:343:ILE:HG13	1:B:345:MET:HE3	1.20	1.11
1:C:81:GLY:HA3	1:D:86:PHE:HZ	1.15	1.09
1:B:73:ALA:HA	1:B:79:LEU:HD11	1.13	1.08
1:B:73:ALA:HA	1:B:79:LEU:CD1	1.90	1.01
1:B:343:ILE:HG13	1:B:345:MET:CE	1.90	1.01
1:C:81:GLY:HA3	1:D:86:PHE:CZ	1.98	0.98
1:C:242:ARG:CG	1:C:242:ARG:HH21	1.77	0.97
1:A:343:ILE:CG1	1:A:345:MET:CE	2.44	0.95
1:B:239:LYS:HG3	4:B:456:HOH:O	1.66	0.93
1:A:343:ILE:HG13	1:A:345:MET:HE3	1.51	0.90
1:C:311:THR:HG23	1:C:326:GLY:HA2	1.55	0.88
1:C:130:ASN:HD21	1:C:143:PHE:H	1.20	0.87
1:C:242:ARG:HG3	1:C:242:ARG:HH21	1.37	0.85
1:B:343:ILE:CG1	1:B:345:MET:HE3	2.04	0.84
1:B:180:LYS:HG3	1:B:206:ASP:HB2	1.60	0.84
1:B:73:ALA:CA	1:B:79:LEU:HD11	2.05	0.83
1:A:343:ILE:HG13	1:A:345:MET:HE1	1.61	0.81
1:A:343:ILE:CG1	1:A:345:MET:HE3	2.08	0.80
1:A:340[A]:ARG:HG3	1:A:340[A]:ARG:HH11	1.47	0.80
1:C:242:ARG:H	1:C:242:ARG:HD2	1.46	0.80
1:B:84:VAL:HG13	1:B:86:PHE:H	1.46	0.79
1:C:81:GLY:CA	1:D:86:PHE:HZ	1.93	0.79
1:D:141:THR:HG23	1:D:160:ASP:OD2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:ASN:HB2	4:D:398:HOH:O	1.86	0.76
1:B:332:LEU:O	1:B:335:LYS:HB3	1.87	0.74
1:D:142:THR:HG23	1:D:155:PHE:CZ	2.22	0.74
1:A:183:GLU:OE2	1:A:190:ARG:HD2	1.88	0.74
1:D:312:GLU:HG3	4:D:364:HOH:O	1.87	0.73
1:A:343:ILE:HG13	1:A:345:MET:HE2	1.68	0.73
1:B:35:LYS:C	1:B:36:LEU:HD12	2.09	0.73
1:B:105:GLN:OE1	1:B:184:PHE:CD1	2.42	0.72
1:B:34:GLU:O	1:B:36:LEU:HD13	1.88	0.72
1:A:170:HIS:HD2	1:A:171:ASP:OD1	1.73	0.72
1:B:35:LYS:O	1:B:36:LEU:HD12	1.89	0.72
1:C:212:THR:HG21	1:C:218:TYR:CD2	2.24	0.72
1:B:187:ASN:O	1:B:188:LYS:HG2	1.89	0.72
1:A:321:LYS:H	1:A:347:ASN:ND2	1.87	0.72
1:D:111:CYS:HB3	1:D:146:VAL:HG12	1.72	0.71
1:D:287:GLY:C	1:D:345:MET:HE3	2.11	0.70
1:A:67:VAL:HG13	1:A:71:ALA:HB3	1.72	0.70
1:C:320:LYS:HA	1:C:347:ASN:ND2	2.06	0.70
1:B:284:VAL:HG13	1:B:348:VAL:HG21	1.74	0.69
1:D:11:VAL:HG22	1:D:16:TRP:CE3	2.28	0.69
1:C:242:ARG:N	1:C:242:ARG:HD2	2.08	0.69
1:C:239:LYS:O	1:D:190:ARG:NH2	2.25	0.68
1:B:239:LYS:HD2	1:B:243:ILE:HD13	1.75	0.68
1:B:187:ASN:C	1:B:188:LYS:HG2	2.14	0.68
1:C:242:ARG:HG3	1:C:242:ARG:NH2	2.09	0.68
1:D:46:THR:O	1:D:50:VAL:HG12	1.94	0.68
1:D:141:THR:CG2	1:D:160:ASP:OD2	2.42	0.67
1:D:325:VAL:O	1:D:325:VAL:HG12	1.96	0.65
1:A:94:SER:HB3	1:A:97:ASP:H	1.61	0.65
1:C:242:ARG:HG2	1:C:242:ARG:HH21	1.60	0.65
1:D:242[A]:ARG:HD3	2:D:354:SO4:S	2.36	0.65
1:A:142:THR:HG22	1:A:155:PHE:CE1	2.32	0.65
1:C:213:THR:HG22	1:C:214:ALA:H	1.61	0.65
1:B:284:VAL:CG1	1:B:348:VAL:HG21	2.26	0.65
1:B:11:VAL:HG22	1:B:16:TRP:CE3	2.32	0.65
1:B:244:ARG:NH2	2:B:353:SO4:O3	2.26	0.65
1:D:212:THR:HG22	4:D:378:HOH:O	1.97	0.64
1:A:84:VAL:HG13	1:A:86:PHE:H	1.62	0.64
1:C:241:ASP:HB3	1:C:242:ARG:HD2	1.79	0.64
1:A:343:ILE:CG1	1:A:345:MET:HE1	2.22	0.64
1:A:72:TRP:O	1:A:74:THR:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340[A]:ARG:HG3	1:A:340[A]:ARG:NH1	2.13	0.63
1:C:64:MET:CE	4:C:389:HOH:O	2.47	0.63
1:B:239:LYS:HD2	1:B:243:ILE:CD1	2.29	0.63
1:D:343:ILE:HG13	1:D:345:MET:CE	2.29	0.63
1:A:72:TRP:C	1:A:74:THR:H	2.02	0.62
1:A:343:ILE:CD1	1:A:345:MET:HE1	2.30	0.61
1:C:64:MET:HE2	4:C:389:HOH:O	1.99	0.61
1:C:42:THR:HG23	1:C:143:PHE:CD1	2.36	0.61
1:B:344:VAL:C	1:B:345:MET:HE2	2.21	0.60
1:A:144:GLN:H	1:A:154:GLN:HE21	1.47	0.60
1:B:267:PRO:O	1:B:268:ASP:HB2	2.01	0.60
1:D:287:GLY:C	1:D:345:MET:CE	2.70	0.59
1:A:339:GLN:O	1:A:340[A]:ARG:HD3	2.03	0.59
1:B:41:LEU:HD11	1:B:219:ASN:HB3	1.85	0.59
1:D:118:VAL:HG21	1:D:125:PHE:HE1	1.68	0.59
1:C:76:ASN:HD22	1:C:76:ASN:N	2.01	0.58
1:D:204:ASN:CB	4:D:398:HOH:O	2.46	0.58
1:D:11:VAL:HG22	1:D:16:TRP:CD2	2.39	0.58
1:D:242[A]:ARG:HD3	2:D:354:SO4:O1	2.04	0.58
1:B:98:LEU:HB3	1:B:114:LEU:HD22	1.84	0.58
1:D:82:SER:HB3	1:D:108:ASN:HD22	1.69	0.58
1:A:70:ASP:OD2	1:A:116:ASP:OD2	2.22	0.57
1:A:264:PRO:HD2	1:A:292:GLY:O	2.04	0.57
1:B:84:VAL:HG13	1:B:86:PHE:N	2.18	0.57
1:B:72:TRP:O	1:B:76:ASN:HB3	2.05	0.57
1:D:118:VAL:HG21	1:D:125:PHE:CE1	2.39	0.57
1:D:168:LEU:HD22	1:D:172:VAL:HG23	1.86	0.57
1:D:174:GLU:HB2	4:D:407:HOH:O	2.05	0.57
1:D:88:LYS:O	1:D:90:GLY:N	2.38	0.57
1:C:320:LYS:HA	1:C:347:ASN:HD22	1.68	0.57
1:A:284:VAL:HG23	1:A:346:GLU:HG3	1.87	0.57
1:D:142:THR:HG23	1:D:155:PHE:CE1	2.40	0.57
1:C:72:TRP:CZ2	1:C:74:THR:HB	2.40	0.56
1:A:262:VAL:HG22	1:A:263:THR:N	2.21	0.56
1:D:180[A]:LYS:HD2	1:D:206:ASP:HA	1.87	0.56
1:D:270:THR:HG22	4:D:368:HOH:O	2.05	0.56
1:A:331:GLN:OE1	1:A:334:GLY:HA2	2.06	0.56
1:A:311:THR:CG2	1:A:326:GLY:HA2	2.36	0.56
1:D:14:ARG:NH2	1:D:34:GLU:OE2	2.39	0.55
1:A:262:VAL:HG22	1:A:263:THR:H	1.71	0.55
1:B:334:GLY:CA	1:B:335:LYS:CB	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:GLN:O	1:C:126:ILE:HG23	2.07	0.55
1:D:325:VAL:CG1	1:D:325:VAL:O	2.54	0.55
1:A:212:THR:O	1:A:212:THR:HG23	2.07	0.55
1:A:84:VAL:HG22	1:A:109:ASP:CG	2.27	0.54
1:B:105:GLN:CG	1:B:184:PHE:HD1	2.20	0.54
1:D:114:LEU:O	1:D:118:VAL:HG22	2.08	0.54
1:C:267:PRO:O	1:C:268:ASP:HB2	2.07	0.54
1:A:272:VAL:HG11	1:A:308:TYR:CZ	2.43	0.54
1:B:169:ILE:CD1	1:B:232:ILE:HD11	2.38	0.53
1:C:212:THR:HG23	2:C:353:SO4:O1	2.09	0.53
1:D:343:ILE:HG13	1:D:345:MET:HE2	1.91	0.53
1:B:105:GLN:CD	1:B:184:PHE:HD1	2.13	0.53
1:B:105:GLN:OE1	1:B:184:PHE:HD1	1.91	0.52
1:D:287:GLY:CA	1:D:345:MET:HE3	2.39	0.52
1:C:242:ARG:HD3	2:D:355:SO4:O3	2.09	0.52
1:B:93:VAL:HG11	1:B:98:LEU:HD13	1.92	0.52
1:D:268:ASP:HB2	4:D:414:HOH:O	2.08	0.52
1:D:126:ILE:HA	1:D:129:MET:HG2	1.92	0.52
1:B:20:ASP:OD2	1:B:261:THR:OG1	2.22	0.52
1:D:45:MET:CG	1:D:129:MET:HB2	2.40	0.52
1:B:334:GLY:HA3	1:B:335:LYS:HB2	0.72	0.52
1:C:16:TRP:HA	1:C:234:VAL:O	2.09	0.51
1:A:311:THR:HG23	1:A:326:GLY:N	2.25	0.51
1:B:35:LYS:C	1:B:36:LEU:CD1	2.78	0.51
1:A:72:TRP:C	1:A:74:THR:N	2.63	0.51
1:D:180[A]:LYS:HD2	1:D:206:ASP:CB	2.40	0.51
1:D:242[A]:ARG:HD3	2:D:354:SO4:O4	2.10	0.51
1:D:55:LYS:HE2	1:D:171:ASP:O	2.11	0.51
1:C:266:LYS:HG3	1:C:267:PRO:HD2	1.93	0.50
1:D:7:GLU:HG2	4:D:382:HOH:O	2.11	0.50
1:C:73:ALA:HB3	1:D:80:ARG:HE	1.76	0.50
1:C:310:LEU:HD23	1:C:325:VAL:HG13	1.91	0.50
1:D:82:SER:HB3	1:D:108:ASN:ND2	2.25	0.50
1:A:317:ALA:HB1	1:A:318:PRO:HA	1.93	0.50
1:D:180[B]:LYS:NZ	1:D:180[B]:LYS:CB	2.75	0.50
1:C:348:VAL:CG2	1:C:348:VAL:O	2.60	0.50
1:A:183:GLU:CD	1:A:190:ARG:HH21	2.15	0.50
1:C:241:ASP:O	1:C:244:ARG:HB3	2.11	0.49
1:D:146:VAL:CG1	1:D:146:VAL:O	2.59	0.49
1:B:97:ASP:OD2	4:B:367:HOH:O	2.20	0.49
1:B:182:LYS:HD2	1:B:199:TRP:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:GLU:CD	1:D:123:GLU:H	2.16	0.49
1:B:244:ARG:HD3	1:B:245:PHE:CE2	2.47	0.49
1:D:41:LEU:HD13	1:D:221:VAL:HG23	1.94	0.49
1:D:343:ILE:HG13	1:D:345:MET:HE1	1.94	0.49
1:D:45:MET:HG2	1:D:129:MET:HB2	1.95	0.49
1:D:288:ALA:N	1:D:345:MET:HE3	2.27	0.49
1:A:84:VAL:HG13	1:A:86:PHE:N	2.26	0.49
1:C:9:PRO:HD3	1:C:254:TRP:CZ2	2.48	0.49
1:C:44:ILE:HG22	1:C:164:LEU:HD13	1.95	0.49
1:B:321:LYS:H	1:B:347:ASN:ND2	2.10	0.49
1:B:187:ASN:O	1:B:188:LYS:CG	2.60	0.48
1:D:296:ILE:HG22	1:D:337:ILE:CD1	2.44	0.48
1:B:12:ASP:OD2	1:B:239:LYS:NZ	2.45	0.48
1:B:284:VAL:CG1	1:B:348:VAL:CG2	2.91	0.48
1:A:311:THR:HG22	1:A:326:GLY:HA2	1.96	0.48
1:A:241:ASP:OD1	1:A:244:ARG:NH2	2.42	0.48
1:A:277:TRP:HB2	1:A:316:THR:HG22	1.95	0.48
1:A:343:ILE:HD11	1:A:345:MET:HE1	1.96	0.48
1:B:133:ALA:HA	1:B:138:LEU:HD22	1.96	0.48
1:C:43:LYS:HE3	1:C:111:CYS:SG	2.53	0.48
1:C:76:ASN:HD22	1:C:76:ASN:H	1.62	0.47
1:C:332:LEU:O	1:C:334:GLY:N	2.47	0.47
1:B:105:GLN:HG3	1:B:184:PHE:HD1	1.79	0.47
1:C:11:VAL:HG22	1:C:16:TRP:CE3	2.50	0.47
1:D:343:ILE:CG1	1:D:345:MET:HE1	2.45	0.47
1:D:141:THR:HG21	1:D:160:ASP:HB3	1.97	0.47
1:C:44:ILE:CG2	1:C:164:LEU:HD13	2.44	0.47
1:B:105:GLN:CD	1:B:184:PHE:CD1	2.88	0.47
1:A:68:GLY:C	1:A:70:ASP:N	2.63	0.47
1:C:212:THR:HG22	1:C:218:TYR:HA	1.96	0.46
1:B:138:LEU:HB3	1:B:141:THR:HB	1.97	0.46
1:C:212:THR:CG2	1:C:218:TYR:CD2	2.96	0.46
1:B:317:ALA:HB1	1:B:318:PRO:HA	1.98	0.46
1:C:65:VAL:O	1:C:92:GLN:HA	2.16	0.46
1:D:102:VAL:O	1:D:106:SER:HA	2.15	0.46
1:A:320:LYS:HA	1:A:347:ASN:HD22	1.81	0.46
1:D:180[A]:LYS:CD	1:D:206:ASP:CB	2.94	0.46
1:C:319:LEU:HB2	1:C:348:VAL:HG22	1.97	0.46
1:A:343:ILE:HG12	1:A:345:MET:HE3	1.94	0.46
1:D:40:SER:HB2	4:D:395:HOH:O	2.14	0.46
1:C:317:ALA:HB1	1:C:318:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:THR:CG2	1:C:326:GLY:HA2	2.35	0.45
1:B:85:MET:O	1:B:86:PHE:HB2	2.17	0.45
1:A:331:GLN:HG2	1:A:336:SER:HA	1.98	0.45
1:D:183:GLU:HG2	1:D:184:PHE:N	2.29	0.45
1:C:27:LEU:HD21	1:C:295:THR:HG21	1.98	0.45
1:B:36:LEU:CD1	1:B:36:LEU:N	2.79	0.45
1:B:187:ASN:HD21	1:C:7:GLU:HG3	1.81	0.45
1:B:11:VAL:HG13	1:B:16:TRP:CE2	2.52	0.45
1:C:325:VAL:O	1:C:325:VAL:HG13	2.17	0.45
1:C:35:LYS:HD3	1:C:155:PHE:CD1	2.51	0.45
1:C:264:PRO:HG2	1:C:330:PHE:CE2	2.52	0.45
1:C:85:MET:O	1:C:86:PHE:HB2	2.16	0.45
1:C:137:GLY:O	1:C:139:THR:HG23	2.17	0.45
1:D:296:ILE:HG22	1:D:337:ILE:HD13	1.99	0.44
1:B:320:LYS:O	1:B:344:VAL:HG22	2.17	0.44
1:B:169:ILE:HD12	1:B:232:ILE:HD11	1.98	0.44
1:C:84:VAL:HG13	1:C:86:PHE:H	1.80	0.44
1:A:233:SER:HB3	1:A:252:LEU:HD13	2.00	0.44
1:A:328:ILE:O	1:A:339:GLN:HA	2.17	0.44
1:C:272:VAL:CG2	1:C:286:LEU:HB2	2.47	0.44
3:A:355:SUC:H1	3:A:355:SUC:H1'2	1.83	0.44
1:C:145:THR:HB	1:C:147:HIS:CE1	2.52	0.44
1:B:128:LEU:HA	1:B:128:LEU:HD12	1.86	0.44
1:C:81:GLY:CA	1:D:86:PHE:CZ	2.82	0.44
1:A:40:SER:O	1:A:43:LYS:HB2	2.17	0.44
1:C:11:VAL:HA	1:C:247:GLU:OE2	2.18	0.44
1:B:343:ILE:CG1	1:B:345:MET:CE	2.78	0.44
1:D:141:THR:CG2	1:D:160:ASP:CB	2.96	0.44
1:C:9:PRO:HD3	1:C:254:TRP:CE2	2.52	0.44
1:A:5:THR:HG23	1:A:6:VAL:N	2.33	0.43
1:C:259:PHE:O	1:C:298[B]:ARG:NH1	2.51	0.43
1:C:242:ARG:H	1:C:242:ARG:CD	2.22	0.43
1:C:212:THR:HG21	1:C:218:TYR:CE2	2.54	0.43
1:A:321:LYS:H	1:A:347:ASN:HD22	1.65	0.43
1:A:142:THR:HG22	1:A:155:PHE:CZ	2.53	0.43
1:C:321:LYS:HG3	1:C:345[B]:MET:O	2.18	0.43
1:D:187:ASN:C	1:D:189:ILE:H	2.22	0.43
1:C:327:THR:HG21	1:C:339:GLN:HE21	1.84	0.43
1:C:236:LEU:HA	1:C:236:LEU:HD12	1.85	0.43
1:C:163:LEU:HA	1:C:163:LEU:HD12	1.89	0.43
1:C:11:VAL:HG13	1:C:16:TRP:CE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:LEU:HD12	1:D:205:VAL:O	2.19	0.42
1:A:14:ARG:NH2	1:A:34:GLU:OE1	2.52	0.42
1:B:244:ARG:HG2	1:B:245:PHE:N	2.30	0.42
1:D:180[A]:LYS:HD2	1:D:206:ASP:CA	2.49	0.42
1:D:56:ALA:O	1:D:57:ASP:CB	2.66	0.42
1:A:332:LEU:HD22	1:A:337:ILE:HD13	2.00	0.42
1:C:242:ARG:NH2	1:C:242:ARG:CG	2.49	0.42
1:C:30:GLY:O	1:C:31:ASN:HB2	2.19	0.42
1:B:239:LYS:H	1:B:239:LYS:HG3	1.62	0.42
1:A:44:ILE:HD11	1:A:209:LYS:HB3	2.02	0.42
1:B:242:ARG:HD3	4:B:422:HOH:O	2.19	0.42
1:D:307:SER:O	1:D:329:ASP:N	2.40	0.42
1:D:271:PHE:HB3	1:D:287:GLY:HA2	2.02	0.42
1:B:76:ASN:OD1	1:B:76:ASN:C	2.58	0.42
1:B:76:ASN:HA	1:B:77:PRO:HD3	1.94	0.42
1:D:88:LYS:C	1:D:90:GLY:H	2.23	0.42
1:D:180[A]:LYS:NZ	4:D:481:HOH:O	2.52	0.42
1:A:343:ILE:O	1:A:345:MET:HE2	2.20	0.42
1:C:39:ALA:HA	1:C:148:GLY:O	2.20	0.41
1:B:25:LYS:HD3	1:B:27:LEU:HD23	2.01	0.41
1:A:311:THR:HG23	1:A:326:GLY:HA2	2.01	0.41
1:C:85:MET:O	1:C:86:PHE:CB	2.68	0.41
1:A:197:LEU:HD12	1:A:197:LEU:HA	1.79	0.41
1:C:309:THR:O	1:C:326:GLY:HA3	2.20	0.41
1:A:265:ILE:O	1:A:292:GLY:HA3	2.20	0.41
1:A:262:VAL:CG2	1:A:263:THR:H	2.33	0.41
1:A:315:LEU:HD12	1:A:315:LEU:HA	1.90	0.41
1:B:320:LYS:HA	1:B:347:ASN:HD22	1.84	0.41
1:A:302:LYS:HB2	1:A:303:ASN:HD22	1.86	0.41
1:B:73:ALA:CA	1:B:79:LEU:CD1	2.81	0.41
1:C:272:VAL:HG23	1:C:286:LEU:HB2	2.03	0.41
1:A:291:ALA:O	1:A:340[A]:ARG:NH1	2.53	0.41
1:C:72:TRP:CE2	1:C:74:THR:HB	2.56	0.41
1:C:257:ARG:O	1:C:298[A]:ARG:HD3	2.20	0.41
1:D:56:ALA:O	1:D:57:ASP:HB2	2.21	0.41
1:D:209:LYS:HB2	1:D:209:LYS:HE3	1.86	0.41
1:B:21:TYR:HB3	1:B:230:ARG:HB3	2.03	0.41
1:C:197:LEU:HA	1:C:197:LEU:HD23	1.87	0.41
1:C:105:GLN:CD	1:C:191:GLN:HG2	2.41	0.41
1:D:141:THR:HG21	1:D:160:ASP:CB	2.50	0.41
1:D:47:SER:HA	1:D:50:VAL:CG1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:TRP:HA	1:A:234:VAL:O	2.21	0.40
1:D:79:LEU:O	1:D:82:SER:HB2	2.21	0.40
1:A:262:VAL:CG2	1:A:263:THR:N	2.85	0.40
1:A:241:ASP:O	1:A:244:ARG:HB3	2.22	0.40
1:D:74:THR:C	1:D:76:ASN:H	2.25	0.40
1:B:180:LYS:HB2	1:B:180:LYS:HE2	1.90	0.40
1:B:180:LYS:HG3	1:B:206:ASP:CB	2.41	0.40
1:C:289:GLY:HA3	1:C:343:ILE:HD11	2.02	0.40
1:D:142:THR:CG2	1:D:155:PHE:CZ	2.99	0.40
1:D:11:VAL:CG2	1:D:16:TRP:CD2	3.04	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	349/352 (99%)	332 (95%)	14 (4%)	3 (1%)	21	15
1	B	346/352 (98%)	330 (95%)	14 (4%)	2 (1%)	30	24
1	C	343/352 (97%)	325 (95%)	17 (5%)	1 (0%)	46	45
1	D	350/352 (99%)	334 (95%)	14 (4%)	2 (1%)	30	24
All	All	1388/1408 (99%)	1321 (95%)	59 (4%)	8 (1%)	30	24

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	335	LYS
1	A	73	ALA
1	A	302	LYS
1	D	89	PRO
1	A	75	GLY

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Mol	Chain	Res	Type
1	B	74	THR
1	D	188	LYS
1	C	152	PRO

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	285/285 (100%)	251 (88%)	34 (12%)	6	3
1	B	282/285 (99%)	252 (89%)	30 (11%)	8	5
1	C	281/285 (99%)	238 (85%)	43 (15%)	3	1
1	D	286/285 (100%)	244 (85%)	42 (15%)	4	2
All	All	1134/1140 (100%)	985 (87%)	149 (13%)	5	2

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	7	GLU
1	A	18	LEU
1	A	40	SER
1	A	43	LYS
1	A	65	VAL
1	A	70	ASP
1	A	83	SER
1	A	84	VAL
1	A	87	LEU
1	A	88	LYS
1	A	94	SER
1	A	123	GLU
1	A	135	LYS
1	A	144	GLN
1	A	163	LEU
1	A	168	LEU
1	A	184	PHE

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Mol	Chain	Res	Type
1	A	188	LYS
1	A	220	LEU
1	A	236	LEU
1	A	246	ASN
1	A	249	GLU
1	A	252	LEU
1	A	272	VAL
1	A	276	VAL
1	A	305	LYS
1	A	307	SER
1	A	311	THR
1	A	319	LEU
1	A	324	VAL
1	A	338	GLU
1	A	348	VAL
1	A	350	GLU
1	B	18	LEU
1	B	57	ASP
1	B	60	LYS
1	B	65	VAL
1	B	88	LYS
1	B	98	LEU
1	B	102	VAL
1	B	128	LEU
1	B	138	LEU
1	B	150	ASP
1	B	163	LEU
1	B	180	LYS
1	B	187	ASN
1	B	188	LYS
1	B	201	SER
1	B	204	ASN
1	B	209	LYS
1	B	220	LEU
1	B	236	LEU
1	B	239	LYS
1	B	242	ARG
1	B	244	ARG
1	B	257	ARG
1	B	268	ASP
1	B	284	VAL
1	B	298	ARG

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Mol	Chain	Res	Type
1	B	302	LYS
1	B	320	LYS
1	B	339	GLN
1	B	340	ARG
1	C	10	SER
1	C	11	VAL
1	C	14	ARG
1	C	18	LEU
1	C	72	TRP
1	C	76	ASN
1	C	80	ARG
1	C	82	SER
1	C	83	SER
1	C	84	VAL
1	C	85	MET
1	C	87	LEU
1	C	98	LEU
1	C	123	GLU
1	C	126	ILE
1	C	128	LEU
1	C	147	HIS
1	C	150	ASP
1	C	163	LEU
1	C	164	LEU
1	C	166	LYS
1	C	168	LEU
1	C	185	THR
1	C	191	GLN
1	C	198	LEU
1	C	204	ASN
1	C	220	LEU
1	C	236	LEU
1	C	242	ARG
1	C	252	LEU
1	C	266	LYS
1	C	274	GLN
1	C	275	ARG
1	C	282	SER
1	C	284	VAL
1	C	294	VAL
1	C	312	GLU
1	C	315	LEU

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Mol	Chain	Res	Type
1	C	319	LEU
1	C	325	VAL
1	C	346	GLU
1	C	348	VAL
1	C	349	GLU
1	D	6	VAL
1	D	40	SER
1	D	50	VAL
1	D	55	LYS
1	D	57	ASP
1	D	64	MET
1	D	69	LYS
1	D	74	THR
1	D	80	ARG
1	D	87	LEU
1	D	92	GLN
1	D	98	LEU
1	D	128	LEU
1	D	134	LYS
1	D	141	THR
1	D	142	THR
1	D	147	HIS
1	D	163	LEU
1	D	168	LEU
1	D	174	GLU
1	D	183	GLU
1	D	184	PHE
1	D	185	THR
1	D	187	ASN
1	D	188	LYS
1	D	198	LEU
1	D	201	SER
1	D	212	THR
1	D	220	LEU
1	D	236	LEU
1	D	239	LYS
1	D	241	ASP
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	270	THR
1	D	275	ARG
1	D	276	VAL

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Mol	Chain	Res	Type
1	D	302	LYS
1	D	305	LYS
1	D	312	GLU
1	D	324	VAL
1	D	339	GLN

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

Mol	Chain	Res	Type
1	A	99	ASN
1	A	154	GLN
1	A	170	HIS
1	A	187	ASN
1	A	303	ASN
1	A	333	ASN
1	A	347	ASN
1	B	144	GLN
1	B	187	ASN
1	B	202	ASN
1	B	204	ASN
1	B	285	ASN
1	B	303	ASN
1	B	347	ASN
1	C	76	ASN
1	C	130	ASN
1	C	204	ASN
1	C	226	GLN
1	C	285	ASN
1	C	303	ASN
1	C	339	GLN
1	C	347	ASN
1	D	105	GLN
1	D	144	GLN
1	D	285	ASN
1	D	303	ASN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	353	-	4,4,4	0.14	0	6,6,6	0.24	0
2	SO4	A	354	-	4,4,4	0.20	0	6,6,6	0.13	0
3	SUC	A	355	-	24,24,24	0.46	0	36,36,36	0.73	0
3	SUC	A	356	-	24,24,24	0.44	0	36,36,36	0.72	0
2	SO4	B	353	-	4,4,4	0.15	0	6,6,6	0.27	0
2	SO4	B	354	-	4,4,4	0.18	0	6,6,6	0.10	0
2	SO4	C	353	-	4,4,4	0.27	0	6,6,6	0.22	0
2	SO4	D	353	-	4,4,4	0.15	0	6,6,6	0.19	0
2	SO4	D	354	-	4,4,4	0.20	0	6,6,6	0.08	0
2	SO4	D	355	-	4,4,4	0.10	0	6,6,6	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	353	-	-	0/0/0/0	0/0/0/0
2	SO4	A	354	-	-	0/0/0/0	0/0/0/0
3	SUC	A	355	-	-	0/12/51/51	0/2/2/2
3	SUC	A	356	-	-	0/12/51/51	0/2/2/2
2	SO4	B	353	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	B	354	-	-	0/0/0/0	0/0/0/0
2	SO4	C	353	-	-	0/0/0/0	0/0/0/0
2	SO4	D	353	-	-	0/0/0/0	0/0/0/0
2	SO4	D	354	-	-	0/0/0/0	0/0/0/0
2	SO4	D	355	-	-	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.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	355	SUC	1	0
2	B	353	SO4	1	0
2	C	353	SO4	1	0
2	D	354	SO4	3	0
2	D	355	SO4	1	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(Å²)	Q<0.9
1	A	348/352 (98%)	0.32	14 (4%)	42	51	19, 35, 64, 80	0
1	B	345/352 (98%)	0.20	10 (2%)	55	63	20, 36, 55, 74	0
1	C	345/352 (98%)	0.36	17 (4%)	33	42	24, 41, 68, 87	0
1	D	350/352 (99%)	0.49	15 (4%)	39	48	22, 37, 72, 99	0
All	All	1388/1408 (98%)	0.34	56 (4%)	42	51	19, 37, 66, 99	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	352	GLY	6.7
1	D	72	TRP	6.6
1	C	74	THR	5.7
1	D	75	GLY	5.7
1	C	73	ALA	5.5
1	D	74	THR	5.4
1	C	215	GLY	5.3
1	D	86	PHE	4.8
1	A	73	ALA	4.6
1	C	86	PHE	4.2
1	C	216	ALA	3.9
1	A	337	ILE	3.8
1	B	352	GLY	3.8
1	A	332	LEU	3.3
1	D	188	LYS	3.3
1	C	80	ARG	3.3
1	A	333	ASN	3.2
1	B	73	ALA	3.2
1	C	77	PRO	3.2
1	A	215	GLY	3.1
1	D	73	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	3.1
1	C	75	GLY	3.0
1	D	77	PRO	3.0
1	C	150	ASP	3.0
1	A	74	THR	3.0
1	B	74	THR	3.0
1	A	72	TRP	3.0
1	D	69	LYS	2.9
1	C	69	LYS	2.8
1	A	352	GLY	2.8
1	A	331	GLN	2.8
1	C	267	PRO	2.7
1	D	333	ASN	2.6
1	D	352	GLY	2.6
1	B	78	ALA	2.6
1	D	80	ARG	2.6
1	B	75	GLY	2.5
1	C	153	GLY	2.5
1	A	214	ALA	2.4
1	B	333	ASN	2.4
1	B	329[A]	ASP	2.4
1	A	155	PHE	2.3
1	D	88	LYS	2.3
1	D	155	PHE	2.3
1	D	78	ALA	2.2
1	A	305	LYS	2.2
1	C	189	ILE	2.2
1	C	214	ALA	2.1
1	A	303	ASN	2.1
1	C	228	ASP	2.1
1	C	268	ASP	2.1
1	D	93	VAL	2.1
1	B	188	LYS	2.0
1	B	330	PHE	2.0
1	B	337	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	B	354	5/5	0.85	0.14	0.66	103,104,105,105	0
2	SO4	D	354	5/5	0.96	0.15	0.35	71,75,76,76	0
2	SO4	B	353	5/5	0.96	0.13	0.04	46,48,52,55	0
2	SO4	D	353	5/5	0.98	0.13	-0.23	55,58,60,63	0
3	SUC	A	356	23/23	0.89	0.12	-0.39	42,53,59,59	0
3	SUC	A	355	23/23	0.90	0.12	-0.52	27,42,47,55	0
2	SO4	C	353	5/5	0.98	0.12	-0.58	50,53,53,57	0
2	SO4	A	353	5/5	0.98	0.09	-1.84	47,50,53,54	0
2	SO4	A	354	5/5	0.96	0.12	-	89,90,90,91	0
2	SO4	D	355	5/5	0.91	0.16	-	63,64,66,68	0

6.5 Other polymers (i)

There are no such residues in this entry.