Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:04 AM GMT

PDB ID	:	2VU2
Title	:	BIOSYNTHETIC THIOLASE FROM Z. RAMIGERA. COMPLEX WITH S -PANTETHEINE-11-PIVALATE.
Authors	:	Kursula, P.; Merilainen, G.; Schmitz, W.; Wierenga, R.K.
Deposited on	:	2008-05-19
Resolution	:	2.65 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:

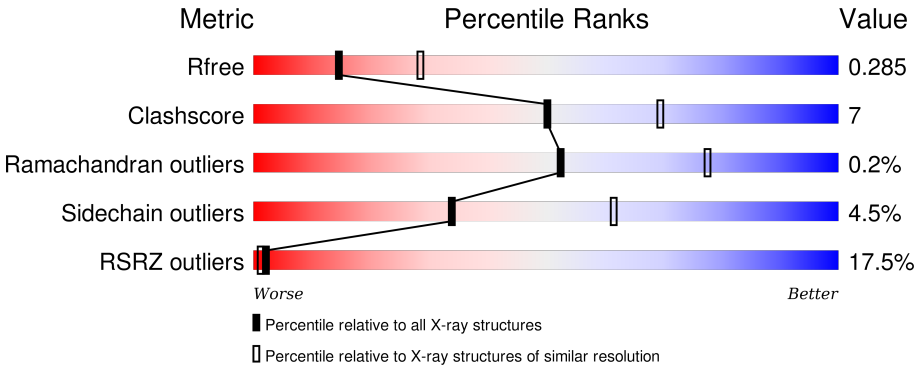
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	392	3% 81% 17%
1	B	392	% 81% 17%
1	C	392	25% 83% 14%
1	D	392	41% 84% 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1396	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11858 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.

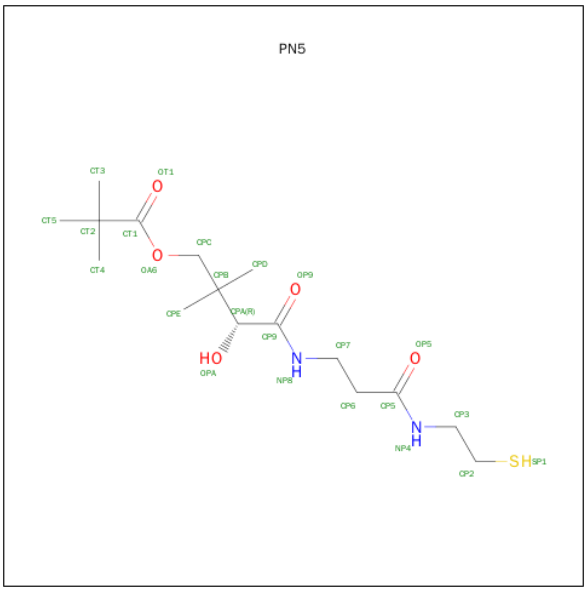
- Molecule 1 is a protein called ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	B	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	C	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	D	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			

There are 4 discrepancies between the modelled and reference sequences:

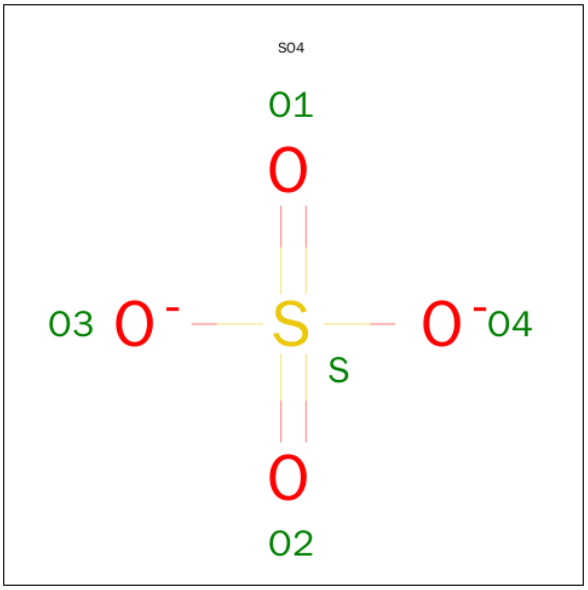
Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ARG	ALA	CONFLICT	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	129	ARG	ALA	CONFLICT	UNP P07097
D	129	ARG	ALA	CONFLICT	UNP P07097

- Molecule 2 is (3R)-3-HYDROXY-2,2-DIMETHYL-4-OXO-4-({3-OXO-3-[(2-SULFANYLETHYL)AMINO]PROPYL}AMINO)BUTYL 2,2-DIMETHYLPROPANOATE (three-letter code: PN5) (formula: $C_{16}H_{30}N_2O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			24	16	2	5	1		
2	B	1	Total	C	N	O	S	0	0
			24	16	2	5	1		

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



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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

- Molecule 4 is water.

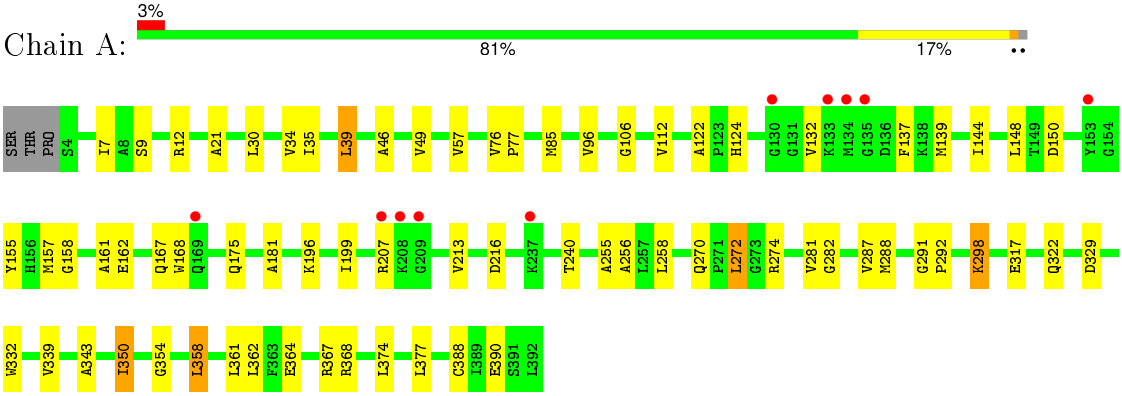
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	240	Total O 240 240	0	0
4	B	228	Total O 228 228	0	0
4	C	36	Total O 36 36	0	0
4	D	24	Total O 24 24	0	0

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.

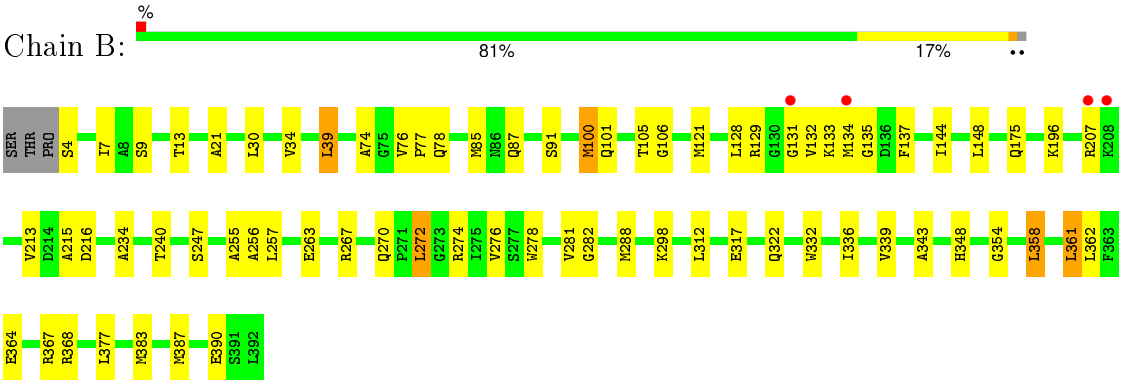
- Molecule 1: ACETYL-COA ACETYLTRANSFERASE

Chain A:



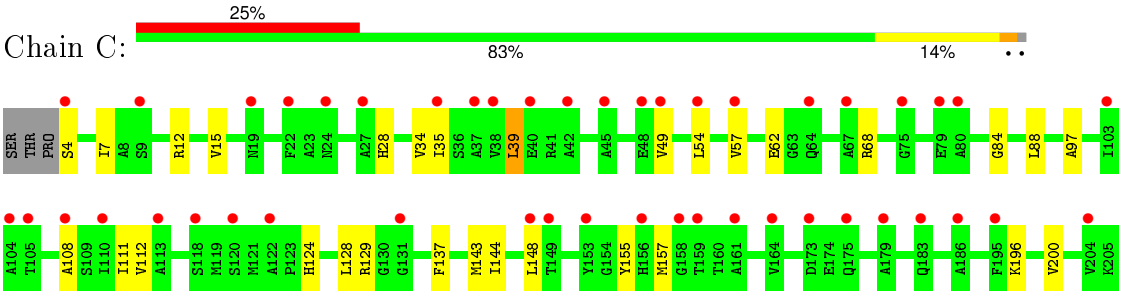
- Molecule 1: ACETYL-COA ACETYLTRANSFERASE

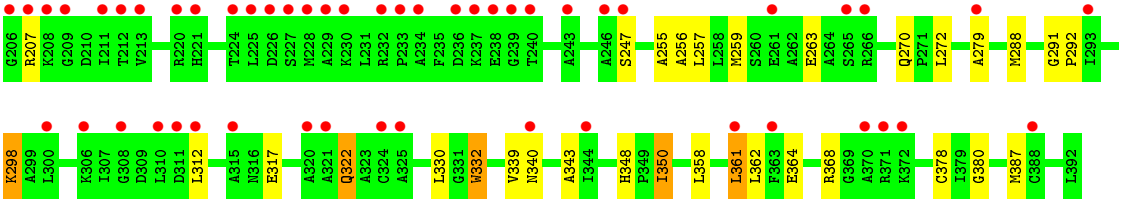
Chain B:



- Molecule 1: ACETYL-COA ACETYLTRANSFERASE

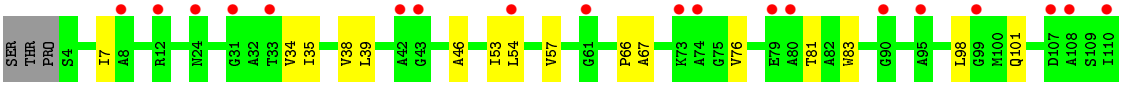
Chain C:

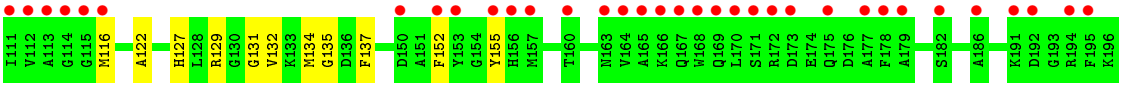


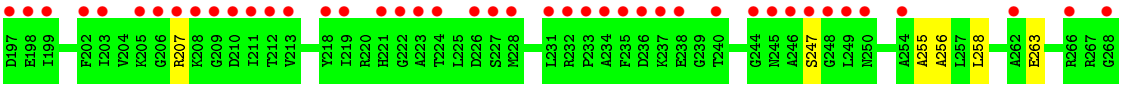


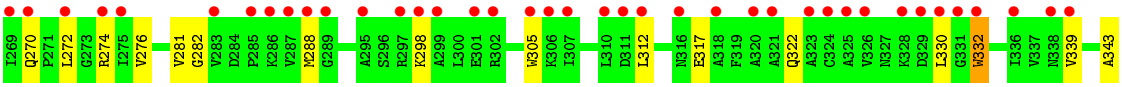
• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

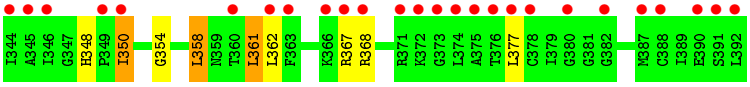
Chain D:











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.32Å 79.15Å 150.79Å 90.00° 92.92° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 19.62 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.3 (20.00-2.65) 82.0 (19.62-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.71 (at 2.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.231 , 0.286 0.236 , 0.285	Depositor DCC
R_{free} test set	2756 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 46.7	EDS
Estimated twinning fraction	0.146 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 55102 reflections	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	11858	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: PN5, 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	0.64	0/2854	0.74	2/3853 (0.1%)
1	B	0.62	0/2854	0.72	3/3853 (0.1%)
1	C	0.36	0/2854	0.52	0/3853
1	D	0.36	0/2854	0.55	2/3853 (0.1%)
All	All	0.51	0/11416	0.64	7/15412 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	367	ARG	NE-CZ-NH2	7.03	123.82	120.30
1	D	367	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	B	367	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	367	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	367	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	100	MET	CG-SD-CE	5.37	108.78	100.20
1	A	367	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	2813	0	2819	47	0
1	B	2813	0	2819	46	0
1	C	2813	0	2819	38	0
1	D	2813	0	2819	37	0
2	A	24	0	30	3	0
2	B	24	0	30	1	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
4	A	240	0	0	6	0
4	B	228	0	0	10	0
4	C	36	0	0	2	0
4	D	24	0	0	1	0
All	All	11858	0	11336	158	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (158) 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:258:LEU:HD22	1:A:258:LEU:N	1.87	0.87
2:A:1393:PN5:HT53	1:D:134:MET:HE1	1.64	0.78
1:D:34:VAL:HG12	1:D:255:ALA:HB3	1.66	0.78
1:C:7:ILE:HD13	1:C:362:LEU:HD11	1.67	0.76
1:C:128:LEU:HD21	1:C:137:PHE:CE2	2.20	0.75
1:D:57:VAL:HG21	1:D:350:ILE:HG22	1.68	0.74
1:B:175:GLN:HE22	1:B:240:THR:CG2	2.03	0.71
1:D:57:VAL:HG21	1:D:350:ILE:CG2	2.21	0.70
1:A:144:ILE:HD13	1:A:148:LEU:HD12	1.73	0.70
1:C:34:VAL:HG12	1:C:255:ALA:HB3	1.74	0.70
1:B:364:GLU:OE2	4:B:2217:HOH:O	2.09	0.69
1:B:128:LEU:HD21	1:B:137:PHE:CE2	2.28	0.68
1:D:339:VAL:HG11	1:D:368:ARG:NH2	2.09	0.67
1:B:274:ARG:NH1	1:B:276:VAL:HG12	2.08	0.67
2:A:1393:PN5:HPE3	4:A:2234:HOH:O	1.96	0.65
1:C:339:VAL:HG11	1:C:368:ARG:NH2	2.12	0.64
1:B:215:ALA:O	4:B:2148:HOH:O	2.15	0.64
1:B:144:ILE:CD1	1:B:148:LEU:HD12	2.27	0.64
1:D:132:VAL:HG21	1:D:137:PHE:CD2	2.32	0.64
2:A:1393:PN5:HT53	1:D:134:MET:CE	2.28	0.62
1:C:257:LEU:HD21	1:C:259:MET:HE2	1.83	0.61
1:B:175:GLN:HE22	1:B:240:THR:HG23	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ALA:O	4:B:2058:HOH:O	2.16	0.60
1:C:7:ILE:HG23	1:C:256:ALA:HB1	1.84	0.60
1:B:312:LEU:HD23	1:B:361:LEU:CD2	2.33	0.59
1:A:34:VAL:HG12	1:A:255:ALA:HB3	1.85	0.59
1:A:258:LEU:CD2	1:A:258:LEU:N	2.65	0.58
1:B:144:ILE:HD13	1:B:148:LEU:HD12	1.85	0.58
1:A:148:LEU:O	1:A:157:MET:HG2	2.03	0.57
1:C:257:LEU:HD21	1:C:259:MET:CE	2.34	0.57
1:B:339:VAL:HG11	1:B:368:ARG:NH2	2.20	0.57
1:C:330:LEU:HD13	1:C:332:TRP:CH2	2.40	0.57
1:B:34:VAL:HG12	1:B:255:ALA:HB3	1.86	0.57
1:C:247:SER:OG	1:C:348:HIS:HB2	2.06	0.56
1:B:234:ALA:HB1	2:B:1393:PN5:HPD2	1.88	0.56
1:B:132:VAL:O	1:D:129:ARG:HA	2.05	0.56
1:A:144:ILE:CD1	1:A:148:LEU:HD12	2.36	0.55
1:D:247:SER:OG	1:D:348:HIS:HB2	2.07	0.55
1:B:196:LYS:NZ	4:B:2133:HOH:O	2.40	0.55
1:A:339:VAL:HG11	1:A:368:ARG:NH2	2.22	0.55
1:D:354:GLY:HA2	1:D:377:LEU:HD21	1.89	0.54
1:B:133:LYS:O	1:D:129:ARG:HD3	2.07	0.54
1:C:57:VAL:HG21	1:C:350:ILE:HG22	1.90	0.54
1:B:312:LEU:HD23	1:B:361:LEU:HD22	1.90	0.54
1:A:57:VAL:HG21	1:A:350:ILE:HG22	1.90	0.54
1:A:175:GLN:HE22	1:A:240:THR:CG2	2.21	0.54
1:B:175:GLN:HE22	1:B:240:THR:HG21	1.71	0.54
1:B:7:ILE:HG23	1:B:256:ALA:HB1	1.90	0.53
1:B:336:ILE:O	1:B:336:ILE:HG13	2.09	0.53
1:D:98:LEU:HD23	1:D:101:GLN:OE1	2.08	0.53
1:D:34:VAL:CG1	1:D:255:ALA:HB3	2.38	0.53
1:A:132:VAL:HG21	1:A:137:PHE:CD2	2.44	0.52
1:A:7:ILE:HG23	1:A:256:ALA:HB1	1.90	0.52
1:C:35:ILE:HG12	1:C:112:VAL:HG11	1.92	0.52
1:D:35:ILE:O	1:D:38:VAL:HG22	2.09	0.52
1:A:258:LEU:HD22	1:A:258:LEU:H	1.73	0.52
1:A:216:ASP:HB3	4:A:2009:HOH:O	2.10	0.52
1:C:54:LEU:O	1:C:84:GLY:HA2	2.10	0.51
1:A:39:LEU:HD11	1:A:49:VAL:CG2	2.40	0.51
1:D:330:LEU:HD13	1:D:332:TRP:CH2	2.46	0.51
1:B:247:SER:OG	1:B:348:HIS:HB2	2.11	0.51
1:D:7:ILE:HD13	1:D:362:LEU:HD11	1.93	0.50
1:C:28:HIS:ND1	1:C:62:GLU:OE2	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ARG:NH2	1:A:390:GLU:OE1	2.44	0.50
1:D:127:HIS:HB3	4:D:2009:HOH:O	2.11	0.50
1:B:267:ARG:HB3	4:B:2171:HOH:O	2.12	0.50
1:C:330:LEU:CD1	1:C:332:TRP:CH2	2.95	0.50
1:A:317:GLU:O	1:A:343:ALA:HB3	2.12	0.50
1:A:9:SER:HA	1:A:272:LEU:HD22	1.93	0.50
1:A:158:GLY:O	1:A:161:ALA:HB3	2.12	0.49
1:B:39:LEU:HD13	1:B:257:LEU:HD12	1.95	0.49
1:A:30:LEU:O	1:A:34:VAL:HG23	2.12	0.49
1:A:85:MET:HA	1:B:85:MET:HA	1.95	0.49
1:B:21:ALA:HB1	1:B:213:VAL:HG21	1.95	0.49
1:A:124:HIS:NE2	1:D:135:GLY:O	2.45	0.49
1:A:122:ALA:HB3	1:B:129:ARG:HH21	1.78	0.48
1:D:66:PRO:HB2	1:D:116:MET:HE3	1.95	0.48
1:B:131:GLY:HA2	1:D:131:GLY:HA2	1.94	0.48
1:C:157:MET:HG3	4:C:2019:HOH:O	2.12	0.48
1:C:57:VAL:HG21	1:C:350:ILE:CG2	2.44	0.48
1:B:78:GLN:HG2	4:B:2065:HOH:O	2.13	0.48
1:D:7:ILE:HG23	1:D:256:ALA:HB1	1.96	0.47
1:C:129:ARG:HH21	1:D:122:ALA:HB3	1.79	0.47
1:D:54:LEU:HD12	1:D:67:ALA:HA	1.96	0.47
1:A:291:GLY:N	1:A:292:PRO:CD	2.77	0.47
1:C:312:LEU:HD23	1:C:361:LEU:CD2	2.44	0.47
1:C:88:LEU:HD12	1:C:380:GLY:O	2.15	0.47
1:B:9:SER:HA	1:B:272:LEU:HD22	1.95	0.47
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.49	0.47
1:B:106:GLY:HA2	4:B:2075:HOH:O	2.15	0.46
1:C:330:LEU:HD13	1:C:332:TRP:CZ3	2.51	0.46
1:D:132:VAL:HG21	1:D:137:PHE:HD2	1.78	0.46
1:A:181:ALA:HB1	4:A:2064:HOH:O	2.14	0.46
1:A:7:ILE:HG12	1:A:258:LEU:HD11	1.96	0.46
1:B:121:MET:HE1	4:B:2021:HOH:O	2.15	0.46
1:A:175:GLN:HE22	1:A:240:THR:HG23	1.81	0.46
1:A:298:LYS:HE3	1:A:298:LYS:HA	1.97	0.46
1:C:257:LEU:CD2	1:C:259:MET:HE2	2.46	0.46
1:C:144:ILE:HD13	1:C:148:LEU:HD12	1.98	0.45
1:C:322:GLN:NE2	1:C:378:CYS:SG	2.89	0.45
1:A:35:ILE:HG12	1:A:112:VAL:HG11	1.97	0.45
1:B:354:GLY:HA2	1:B:377:LEU:HD21	1.98	0.45
1:A:374:LEU:HD12	1:A:388:CYS:SG	2.57	0.45
1:B:135:GLY:O	1:C:124:HIS:NE2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ALA:HB2	1:C:387:MET:CE	2.46	0.45
1:B:358:LEU:HD22	1:B:362:LEU:HG	1.99	0.45
1:D:57:VAL:HG21	1:D:350:ILE:HG21	1.99	0.44
1:A:46:ALA:HB1	1:A:76:VAL:HA	1.99	0.44
1:D:312:LEU:HD23	1:D:361:LEU:CD2	2.48	0.44
1:B:134:MET:HG3	1:C:143:MET:HE1	2.00	0.44
1:A:21:ALA:HB1	1:A:213:VAL:HG21	2.00	0.44
1:C:279:ALA:HB1	1:C:298:LYS:HB3	1.98	0.44
1:A:139:MET:HG3	1:D:137:PHE:CE1	2.53	0.44
1:D:281:VAL:HG12	1:D:282:GLY:N	2.33	0.44
1:C:68:ARG:HG3	1:D:152:PHE:HZ	1.83	0.43
1:A:96:VAL:HG21	1:A:358:LEU:HD12	2.00	0.43
1:A:281:VAL:HG12	1:A:282:GLY:N	2.33	0.43
1:B:274:ARG:HH12	1:B:276:VAL:HG12	1.81	0.43
1:D:276:VAL:HG21	1:D:305:TRP:CZ2	2.53	0.43
1:B:76:VAL:HG13	1:B:77:PRO:HD2	2.01	0.43
1:D:274:ARG:NH1	1:D:276:VAL:HG12	2.34	0.43
1:D:7:ILE:HG12	1:D:258:LEU:CD1	2.49	0.42
1:C:340:ASN:ND2	1:C:364:GLU:OE1	2.47	0.42
1:D:46:ALA:HB1	1:D:76:VAL:HA	2.01	0.42
1:A:377:LEU:N	1:A:377:LEU:HD12	2.35	0.42
1:A:162:GLU:OE1	1:A:240:THR:HG22	2.19	0.42
1:C:108:ALA:CB	1:C:111:ILE:HD11	2.49	0.42
1:A:7:ILE:HD13	1:A:362:LEU:HD11	2.02	0.42
1:B:216:ASP:HB3	4:B:2213:HOH:O	2.18	0.42
1:B:281:VAL:HG12	1:B:282:GLY:N	2.35	0.42
1:D:317:GLU:O	1:D:343:ALA:HB3	2.19	0.42
1:B:274:ARG:NH2	1:B:390:GLU:OE1	2.52	0.42
1:C:196:LYS:NZ	4:C:2024:HOH:O	2.52	0.42
1:A:76:VAL:CG1	1:A:77:PRO:HD2	2.50	0.41
1:A:106:GLY:HA2	4:A:2085:HOH:O	2.20	0.41
1:B:101:GLN:O	1:B:105:THR:HG23	2.20	0.41
1:C:317:GLU:O	1:C:343:ALA:HB3	2.20	0.41
1:C:257:LEU:CD2	1:C:259:MET:CE	2.98	0.41
1:B:317:GLU:O	1:B:343:ALA:HB3	2.20	0.41
1:C:257:LEU:C	1:C:257:LEU:HD23	2.41	0.41
1:A:354:GLY:HA2	1:A:377:LEU:HD21	2.03	0.41
1:C:39:LEU:HD11	1:C:49:VAL:CG2	2.51	0.41
1:B:278:TRP:HA	1:B:387:MET:HA	2.02	0.41
1:B:383:MET:HE2	4:B:2221:HOH:O	2.20	0.41
1:C:200:VAL:HG13	1:C:200:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:VAL:O	1:D:38:VAL:HG13	2.21	0.41
1:B:87:GLN:N	1:B:91:SER:OG	2.50	0.41
1:D:53:ILE:HD13	1:D:83:TRP:CZ2	2.56	0.41
1:A:167:GLN:OE1	1:A:287:VAL:HG11	2.21	0.41
1:B:13:THR:HG21	1:B:30:LEU:HD22	2.03	0.41
1:A:150:ASP:OD1	4:A:2110:HOH:O	2.22	0.41
1:A:364:GLU:O	1:A:368:ARG:HG2	2.21	0.40
1:D:358:LEU:HD22	1:D:362:LEU:HG	2.04	0.40
1:A:196:LYS:NZ	4:A:2139:HOH:O	2.37	0.40
1:C:291:GLY:N	1:C:292:PRO:CD	2.84	0.40
1:A:12:ARG:O	1:A:199:ILE:HA	2.21	0.40
1:A:57:VAL:HG21	1:A:350:ILE:CG2	2.51	0.40
1:C:12:ARG:HH12	1:C:15:VAL:HG23	1.87	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	387/392 (99%)	369 (95%)	17 (4%)	1 (0%)	46	72
1	B	387/392 (99%)	366 (95%)	21 (5%)	0	100	100
1	C	387/392 (99%)	372 (96%)	14 (4%)	1 (0%)	46	72
1	D	387/392 (99%)	374 (97%)	12 (3%)	1 (0%)	46	72
All	All	1548/1568 (99%)	1481 (96%)	64 (4%)	3 (0%)	52	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	350	ILE
1	D	350	ILE

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Mol	Chain	Res	Type
1	A	350	ILE

5.3.2 Protein sidechains

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	276/279 (99%)	265 (96%)	11 (4%)	38	66
1	B	276/279 (99%)	263 (95%)	13 (5%)	32	60
1	C	276/279 (99%)	263 (95%)	13 (5%)	32	60
1	D	276/279 (99%)	263 (95%)	13 (5%)	32	60
All	All	1104/1116 (99%)	1054 (96%)	50 (4%)	34	61

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

Mol	Chain	Res	Type
1	A	39	LEU
1	A	155	TYR
1	A	207	ARG
1	A	270	GLN
1	A	272	LEU
1	A	288	MET
1	A	298	LYS
1	A	322	GLN
1	A	332	TRP
1	A	358	LEU
1	A	361	LEU
1	B	4	SER
1	B	39	LEU
1	B	100	MET
1	B	207	ARG
1	B	263	GLU
1	B	270	GLN
1	B	272	LEU
1	B	288	MET
1	B	298	LYS

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Mol	Chain	Res	Type
1	B	322	GLN
1	B	332	TRP
1	B	358	LEU
1	B	361	LEU
1	C	4	SER
1	C	39	LEU
1	C	155	TYR
1	C	207	ARG
1	C	263	GLU
1	C	270	GLN
1	C	272	LEU
1	C	288	MET
1	C	298	LYS
1	C	322	GLN
1	C	332	TRP
1	C	358	LEU
1	C	361	LEU
1	D	39	LEU
1	D	81	THR
1	D	155	TYR
1	D	207	ARG
1	D	263	GLU
1	D	270	GLN
1	D	272	LEU
1	D	288	MET
1	D	298	LYS
1	D	322	GLN
1	D	332	TRP
1	D	358	LEU
1	D	361	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	156	HIS
1	A	175	GLN
1	A	184	ASN
1	B	78	GLN
1	B	156	HIS
1	B	175	GLN
1	B	184	ASN

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Mol	Chain	Res	Type
1	C	78	GLN
1	C	184	ASN
1	C	270	GLN
1	C	316	ASN
1	C	322	GLN
1	D	78	GLN
1	D	175	GLN
1	D	184	ASN
1	D	316	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)

8 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	PN5	A	1393	-	20,23,23	1.29	1 (5%)	27,32,32	1.49	6 (22%)
3	SO4	A	1394	-	4,4,4	0.22	0	6,6,6	0.24	0
3	SO4	A	1395	-	4,4,4	0.13	0	6,6,6	0.17	0
3	SO4	A	1396	-	4,4,4	0.21	0	6,6,6	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PN5	B	1393	-	20,23,23	1.31	1 (5%)	27,32,32	1.95	7 (25%)
3	SO4	B	1394	-	4,4,4	0.21	0	6,6,6	0.14	0
3	SO4	B	1395	-	4,4,4	0.21	0	6,6,6	0.39	0
3	SO4	B	1396	-	4,4,4	0.10	0	6,6,6	0.41	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	PN5	A	1393	-	-	0/32/32/32	0/0/0/0
3	SO4	A	1394	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1395	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1396	-	-	0/0/0/0	0/0/0/0
2	PN5	B	1393	-	-	0/32/32/32	0/0/0/0
3	SO4	B	1394	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1395	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1396	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1393	PN5	OA6-CT1	5.41	1.46	1.33
2	B	1393	PN5	OA6-CT1	5.48	1.46	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1393	PN5	CP2-CP3-NP4	-3.52	105.43	112.37
2	A	1393	PN5	CP2-CP3-NP4	-3.08	106.29	112.37
2	B	1393	PN5	OA6-CT1-OT1	-3.04	117.74	124.44
2	B	1393	PN5	CP6-CP7-NP8	-2.97	105.36	111.88
2	A	1393	PN5	OA6-CT1-OT1	-2.38	119.21	124.44
2	A	1393	PN5	CPD-CPB-CPC	2.18	111.32	108.50
2	A	1393	PN5	CP7-NP8-CP9	2.74	127.96	122.53
2	A	1393	PN5	CPC-OA6-CT1	2.88	121.10	116.97
2	B	1393	PN5	CP3-NP4-CP5	3.10	128.88	122.79
2	A	1393	PN5	OA6-CT1-CT2	3.32	119.67	112.79
2	B	1393	PN5	CP7-NP8-CP9	3.49	129.44	122.53
2	B	1393	PN5	OA6-CT1-CT2	3.69	120.44	112.79
2	B	1393	PN5	CPC-OA6-CT1	4.72	123.72	116.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1393	PN5	3	0
2	B	1393	PN5	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	389/392 (99%)	0.07	10 (2%) 59 58	69, 78, 90, 105	0
1	B	389/392 (99%)	0.09	4 (1%) 84 84	69, 78, 89, 107	0
1	C	389/392 (99%)	1.44	97 (24%) 1 1	65, 80, 92, 98	0
1	D	389/392 (99%)	1.99	161 (41%) 0 0	67, 81, 95, 101	0
All	All	1556/1568 (99%)	0.90	272 (17%) 2 1	65, 79, 92, 107	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	331	GLY	13.0
1	D	371	ARG	8.7
1	D	228	MET	8.6
1	D	157	MET	8.4
1	D	231	LEU	7.2
1	C	243	ALA	6.5
1	D	238	GLU	6.4
1	C	80	ALA	6.3
1	D	367	ARG	6.1
1	D	269	ILE	6.0
1	D	219	ILE	5.9
1	D	226	ASP	5.8
1	D	173	ASP	5.8
1	D	170	LEU	5.4
1	C	315	ALA	5.2
1	D	320	ALA	5.1
1	D	368	ARG	5.1
1	C	221	HIS	5.0
1	D	362	LEU	5.0
1	D	245	ASN	5.0
1	D	153	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	232	ARG	5.0
1	C	204	VAL	4.9
1	C	57	VAL	4.8
1	C	208	LYS	4.7
1	D	240	THR	4.6
1	D	330	LEU	4.6
1	C	236	ASP	4.5
1	C	370	ALA	4.5
1	D	166	LYS	4.4
1	C	232	ARG	4.4
1	D	207	ARG	4.4
1	C	186	ALA	4.3
1	D	73	LYS	4.3
1	D	222	GLY	4.3
1	D	388	CYS	4.3
1	D	167	GLN	4.2
1	D	235	PHE	4.1
1	D	268	GLY	4.1
1	C	213	VAL	4.1
1	C	156	HIS	4.1
1	D	310	LEU	4.1
1	C	226	ASP	4.1
1	C	246	ALA	4.1
1	D	208	LYS	4.1
1	D	246	ALA	4.0
1	D	244	GLY	4.0
1	D	152	PHE	4.0
1	D	191	LYS	4.0
1	D	262	ALA	4.0
1	D	221	HIS	3.9
1	C	320	ALA	3.9
1	C	321	ALA	3.9
1	D	206	GLY	3.9
1	C	173	ASP	3.8
1	C	164	VAL	3.8
1	D	374	LEU	3.7
1	D	61	GLY	3.7
1	A	208	LYS	3.7
1	C	110	ILE	3.7
1	D	349	PRO	3.7
1	D	318	ALA	3.7
1	C	220	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	233	PRO	3.7
1	C	308	GLY	3.7
1	D	328	LYS	3.6
1	C	131	GLY	3.6
1	D	289	GLY	3.6
1	C	67	ALA	3.6
1	D	378	CYS	3.6
1	D	42	ALA	3.5
1	C	159	THR	3.5
1	C	9	SER	3.5
1	C	227	SER	3.5
1	D	165	ALA	3.5
1	D	156	HIS	3.5
1	D	323	ALA	3.5
1	D	218	TYR	3.5
1	D	301	GLU	3.5
1	D	312	LEU	3.4
1	D	31	GLY	3.4
1	D	288	MET	3.4
1	C	179	ALA	3.4
1	C	207	ARG	3.4
1	D	387	MET	3.4
1	D	286	LYS	3.4
1	D	329	ASP	3.4
1	D	150	ASP	3.3
1	D	285	PRO	3.3
1	D	168	TRP	3.3
1	D	298	LYS	3.3
1	D	373	GLY	3.3
1	C	104	ALA	3.3
1	D	324	CYS	3.3
1	C	230	LYS	3.3
1	D	182	SER	3.3
1	D	99	GLY	3.3
1	D	336	ILE	3.3
1	C	212	THR	3.2
1	D	237	LYS	3.2
1	D	233	PRO	3.2
1	C	224	THR	3.2
1	D	295	ALA	3.2
1	B	208	LYS	3.2
1	D	326	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	371	ARG	3.2
1	C	149	THR	3.2
1	C	211	ILE	3.1
1	D	205	LYS	3.1
1	D	107	ASP	3.1
1	D	79	GLU	3.1
1	D	194	ARG	3.1
1	C	311	ASP	3.1
1	D	249	LEU	3.1
1	D	372	LYS	3.1
1	C	229	ALA	3.0
1	D	175	GLN	3.0
1	D	321	ALA	3.0
1	D	366	LYS	3.0
1	D	169	GLN	3.0
1	D	43	GLY	3.0
1	D	202	PHE	3.0
1	C	266	ARG	2.9
1	C	161	ALA	2.9
1	D	186	ALA	2.9
1	D	12	ARG	2.9
1	C	325	ALA	2.9
1	D	302	ARG	2.9
1	D	164	VAL	2.8
1	D	171	SER	2.8
1	D	177	ALA	2.8
1	C	225	LEU	2.8
1	D	350	ILE	2.8
1	D	382	GLY	2.8
1	D	377	LEU	2.8
1	C	265	SER	2.8
1	C	310	LEU	2.8
1	B	131	GLY	2.8
1	C	79	GLU	2.7
1	C	183	GLN	2.7
1	D	332	TRP	2.7
1	D	172	ARG	2.7
1	D	209	GLY	2.7
1	C	238	GLU	2.7
1	C	19	ASN	2.7
1	D	316	ASN	2.7
1	D	155	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	213	VAL	2.7
1	A	134	MET	2.7
1	D	95	ALA	2.7
1	D	272	LEU	2.7
1	D	236	ASP	2.7
1	C	42	ALA	2.7
1	C	240	THR	2.7
1	D	33	THR	2.7
1	C	237	LYS	2.6
1	D	114	GLY	2.6
1	C	103	ILE	2.6
1	D	248	GLY	2.6
1	C	340	ASN	2.6
1	C	45	ALA	2.6
1	D	179	ALA	2.6
1	D	254	ALA	2.6
1	D	198	GLU	2.6
1	B	207	ARG	2.6
1	C	306	LYS	2.6
1	C	312	LEU	2.6
1	C	293	ILE	2.6
1	C	105	THR	2.5
1	D	360	THR	2.5
1	D	212	THR	2.5
1	C	209	GLY	2.5
1	B	134	MET	2.5
1	C	4	SER	2.5
1	C	40	GLU	2.5
1	C	195	PHE	2.5
1	C	361	LEU	2.5
1	C	153	TYR	2.5
1	D	90	GLY	2.5
1	D	234	ALA	2.5
1	C	388	CYS	2.5
1	C	363	PHE	2.5
1	C	300	LEU	2.4
1	D	111	ILE	2.4
1	D	287	VAL	2.4
1	A	209	GLY	2.4
1	D	108	ALA	2.4
1	D	197	ASP	2.4
1	D	24	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	206	GLY	2.4
1	D	375	ALA	2.4
1	D	199	ILE	2.4
1	C	24	ASN	2.4
1	D	297	ARG	2.4
1	D	311	ASP	2.4
1	D	376	THR	2.4
1	D	163	ASN	2.4
1	D	250	ASN	2.4
1	D	74	ALA	2.3
1	D	113	ALA	2.3
1	C	261	GLU	2.3
1	C	279	ALA	2.3
1	D	339	VAL	2.3
1	C	324	CYS	2.3
1	D	178	PHE	2.3
1	D	211	ILE	2.3
1	A	135	GLY	2.3
1	C	108	ALA	2.3
1	D	299	ALA	2.3
1	D	305	TRP	2.3
1	D	325	ALA	2.3
1	D	363	PHE	2.3
1	C	247	SER	2.3
1	D	306	LYS	2.3
1	C	372	LYS	2.3
1	D	210	ASP	2.3
1	D	247	SER	2.3
1	C	122	ALA	2.3
1	D	338	ASN	2.3
1	D	160	THR	2.3
1	D	270	GLN	2.3
1	C	120	SER	2.2
1	D	274	ARG	2.2
1	D	195	PHE	2.2
1	A	130	GLY	2.2
1	D	275	ILE	2.2
1	A	169	GLN	2.2
1	C	228	MET	2.2
1	D	203	ILE	2.2
1	D	344	ILE	2.2
1	D	192	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	49	VAL	2.2
1	D	112	VAL	2.2
1	C	175	GLN	2.2
1	C	37	ALA	2.2
1	D	283	VAL	2.2
1	C	344	ILE	2.2
1	D	223	ALA	2.2
1	D	80	ALA	2.1
1	D	307	ILE	2.1
1	D	346	ILE	2.1
1	C	239	GLY	2.1
1	D	380	GLY	2.1
1	C	148	LEU	2.1
1	C	54	LEU	2.1
1	D	392	LEU	2.1
1	A	237	LYS	2.1
1	D	390	GLU	2.1
1	A	153	TYR	2.1
1	C	75	GLY	2.1
1	C	64	GLN	2.1
1	A	133	LYS	2.1
1	C	27	ALA	2.1
1	C	234	ALA	2.1
1	C	118	SER	2.1
1	D	224	THR	2.1
1	C	35	ILE	2.1
1	C	158	GLY	2.1
1	D	115	GLY	2.1
1	D	227	SER	2.0
1	D	345	ALA	2.0
1	D	54	LEU	2.0
1	C	38	VAL	2.0
1	C	22	PHE	2.0
1	D	116	MET	2.0
1	D	391	SER	2.0
1	C	48	GLU	2.0
1	D	110	ILE	2.0
1	C	113	ALA	2.0
1	D	8	ALA	2.0
1	A	207	ARG	2.0
1	D	266	ARG	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
3	SO4	A	1396	5/5	0.96	0.30	4.02	69,72,74,77	0
2	PN5	B	1393	24/24	0.83	0.27	2.00	70,86,91,94	0
3	SO4	B	1396	5/5	0.97	0.27	1.94	66,66,68,69	0
2	PN5	A	1393	24/24	0.87	0.24	1.93	72,75,81,83	0
3	SO4	B	1395	5/5	0.96	0.29	-	70,73,75,77	0
3	SO4	A	1395	5/5	0.92	0.32	-	91,91,92,93	0
3	SO4	A	1394	5/5	0.94	0.32	-	79,81,82,83	0
3	SO4	B	1394	5/5	0.90	0.26	-	95,96,96,96	0

6.5 Other polymers (i)

There are no such residues in this entry.