Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:39 AM GMT

PDB ID	:	3MEC
Title	:	HIV-1 Reverse Transcriptase in Complex with TMC125
Authors	:	Lansdon, E.B.
Deposited on	:	2010-03-31
Resolution	:	2.30 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:

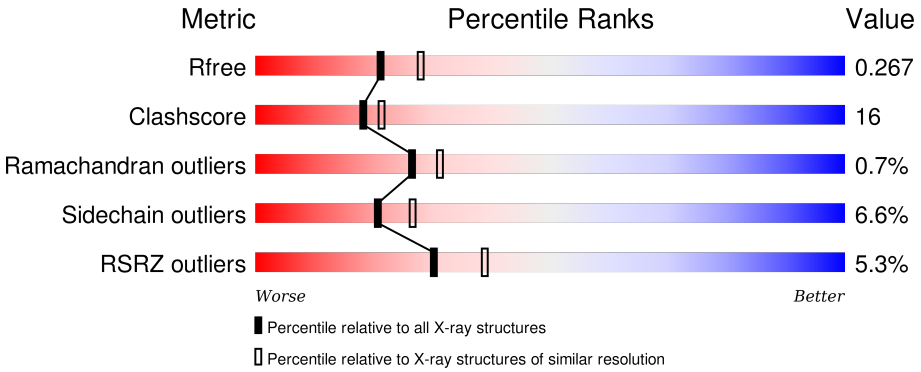
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	560	4% 67% 27% 5%
2	B	440	6% 63% 26% 9%

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
4	SO4	A	564	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8072 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.

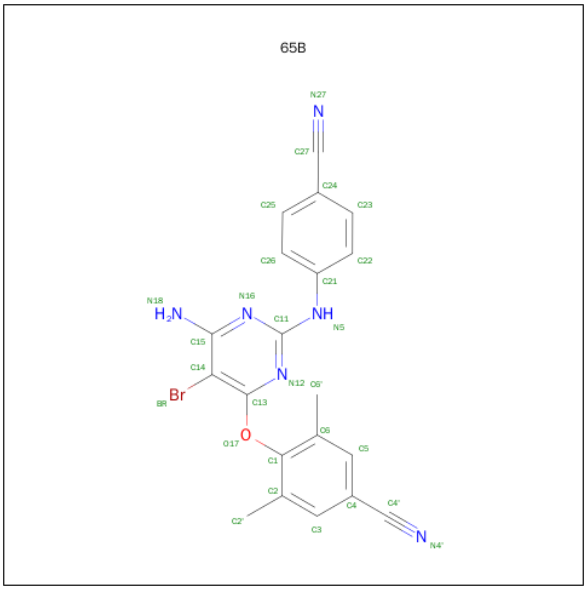
- Molecule 1 is a protein called p66 Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4483	2900	746	829	8			

- Molecule 2 is a protein called p51 Reverse transcriptase.

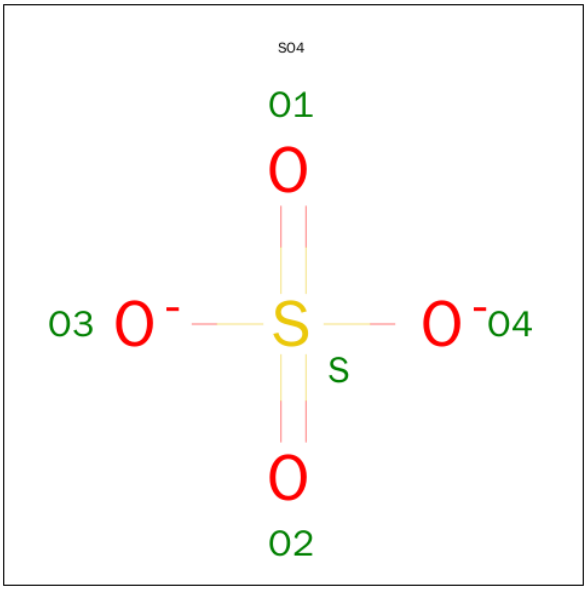
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3321	2164	548	603	6			

- Molecule 3 is 4-({6-AMINO-5-BROMO-2-[(4-CYANOPHENYL)AMINO]PYRIMIDIN-4-YL}OXY)-3,5-DIMETHYLBENZONITRILE (three-letter code: 65B) (formula: $C_{20}H_{15}BrN_6O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			28	1	20	6	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

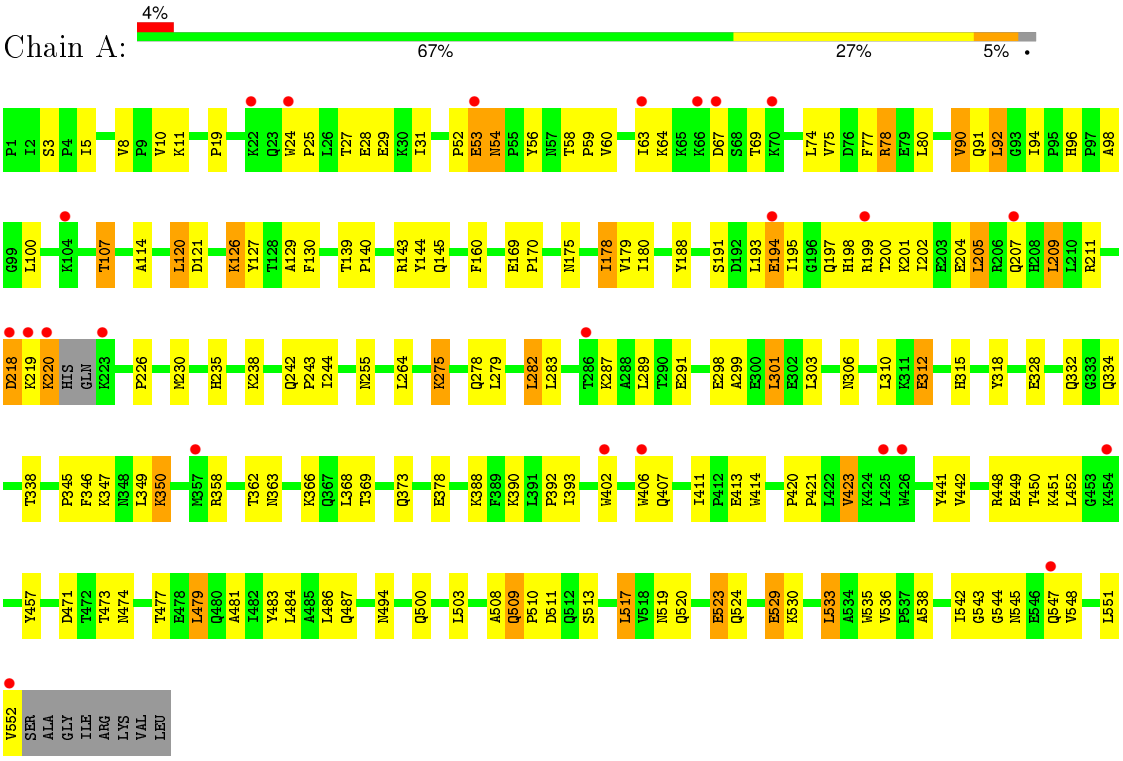
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	125	Total O 125 125	0	0
5	B	90	Total O 90 90	0	0

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.

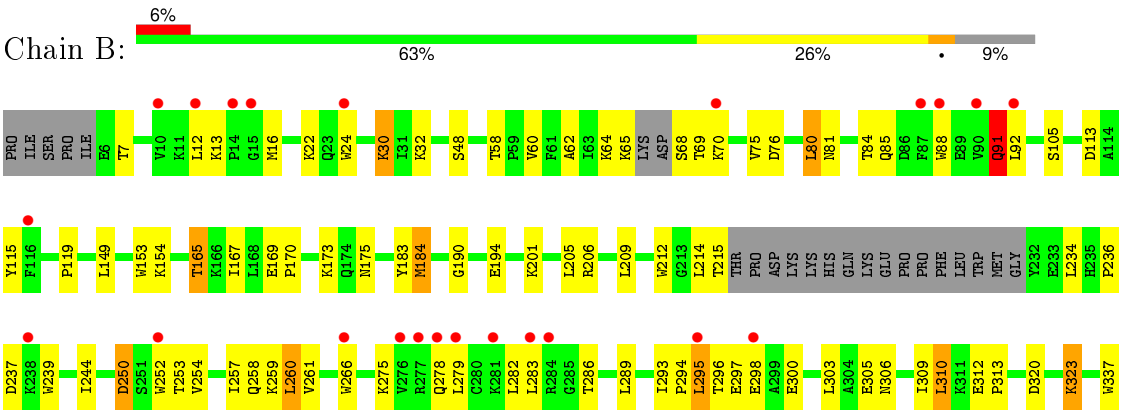
- Molecule 1: p66 Reverse transcriptase

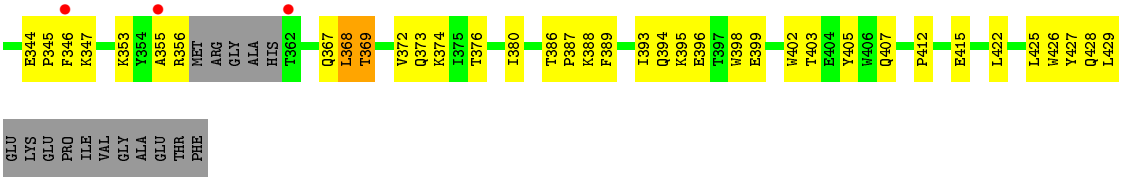
Chain A:



- Molecule 2: p51 Reverse transcriptase

Chain B:




E344
P345
F346
K347
K353
Y354
A355
R356
MET
ARG
GLY
ALA
HIS
T362
Q367
L368
T369
V372
Q373
K374
I375
T376
I380
T386
P387
K388
F389
I393
Q394
K395
E396
T397
W398
E399
W402
T403
E404
Y405
W406
Q407
P412
E415
L422
L425
W426
Y427
Q428
L429
GLU
LYS
GLU
PRO
ILE
VAL
GLY
ALA
GLU
THR
PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	118.95Å 154.12Å 154.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 2.30 47.16 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.6 (29.91-2.30) 90.7 (47.16-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.81 (at 2.32Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.226 , 0.270 0.224 , 0.267	Depositor DCC
R_{free} test set	2878 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.1	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 61973 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8072	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: 65B, 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	0.33	0/4598	0.50	0/6246
2	B	0.34	0/3413	0.50	0/4637
All	All	0.33	0/8011	0.50	0/10883

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	91	GLN	Peptide

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	4483	0	4537	150	0
2	B	3321	0	3352	103	0
3	A	28	0	15	2	0
4	A	20	0	0	0	0
4	B	5	0	0	1	0
5	A	125	0	0	7	0
5	B	90	0	0	2	0
All	All	8072	0	7904	246	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 16.

All (246) 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:90:VAL:HG23	1:A:91:GLN:H	1.30	0.97
2:B:260:LEU:HD13	2:B:279:LEU:HD21	1.53	0.87
1:A:52:PRO:HA	1:A:53:GLU:C	1.95	0.87
1:A:92:LEU:H	1:A:92:LEU:HD23	1.44	0.82
1:A:451:LYS:HB3	1:A:471:ASP:HA	1.62	0.82
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.61	0.80
1:A:275:LYS:H	1:A:306:ASN:HD21	1.25	0.80
1:A:194:GLU:H	1:A:194:GLU:CD	1.89	0.76
1:A:520:GLN:O	1:A:523:GLU:HG3	1.87	0.75
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.68	0.75
2:B:296:THR:HG22	2:B:298:GLU:H	1.52	0.74
1:A:503:LEU:HD13	1:A:533:LEU:HD12	1.69	0.74
2:B:297:GLU:HG3	2:B:298:GLU:H	1.53	0.74
2:B:259:LYS:HE2	2:B:425:LEU:HD21	1.70	0.73
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.34	0.72
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.69	0.72
1:A:199:ARG:HG2	1:A:199:ARG:HH11	1.52	0.72
1:A:298:GLU:H	1:A:298:GLU:CD	1.93	0.72
1:A:64:LYS:NZ	1:A:69:THR:HG22	2.05	0.72
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.73	0.71
1:A:96:HIS:HD1	1:A:98:ALA:H	1.39	0.70
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.73	0.70
2:B:69:THR:O	2:B:70:LYS:HG3	1.92	0.70
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.74	0.70
1:A:450:THR:HG22	1:A:452:LEU:HB2	1.73	0.69
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.08	0.69
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:ASN:ND2	2:B:154:LYS:H	1.91	0.68
2:B:295:LEU:H	2:B:295:LEU:HD22	1.58	0.68
1:A:503:LEU:HD23	2:B:422:LEU:HD21	1.76	0.68
2:B:376:THR:HG23	2:B:386:THR:HG23	1.75	0.68
1:A:64:LYS:HZ3	1:A:69:THR:HA	1.60	0.67
1:A:191:SER:HB2	1:A:193:LEU:HD23	1.78	0.66
1:A:479:LEU:HB3	1:A:517:LEU:HD13	1.79	0.65
2:B:312:GLU:HB3	2:B:313:PRO:HD2	1.79	0.64
2:B:373:GLN:HE22	2:B:407:GLN:H	1.44	0.64
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.80	0.64
1:A:406:TRP:HE3	1:A:407:GLN:HE21	1.46	0.63
1:A:27:THR:HG22	1:A:29:GLU:H	1.62	0.63
1:A:486:LEU:HB3	1:A:524:GLN:HG3	1.81	0.63
2:B:252:TRP:CD1	2:B:295:LEU:HD11	2.33	0.63
1:A:90:VAL:HG23	1:A:91:GLN:N	2.09	0.63
2:B:373:GLN:NE2	2:B:407:GLN:H	1.97	0.62
1:A:175:ASN:HB3	1:A:178:ILE:CG2	2.29	0.62
1:A:169:GLU:HB2	1:A:170:PRO:HD3	1.82	0.62
2:B:297:GLU:HG3	2:B:298:GLU:N	2.15	0.61
1:A:64:LYS:HZ1	1:A:69:THR:HG22	1.63	0.61
1:A:334:GLN:HB3	5:A:611:HOH:O	1.99	0.61
1:A:509:GLN:N	1:A:510:PRO:HD3	2.16	0.61
1:A:175:ASN:HD22	1:A:201:LYS:NZ	1.99	0.60
2:B:293:ILE:HG13	2:B:294:PRO:HD2	1.82	0.60
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.02	0.60
1:A:175:ASN:ND2	1:A:201:LYS:NZ	2.49	0.60
1:A:197:GLN:O	1:A:201:LYS:HG2	2.02	0.60
2:B:13:LYS:HB2	2:B:16:MET:SD	2.41	0.60
2:B:295:LEU:HD22	2:B:295:LEU:N	2.17	0.59
2:B:32:LYS:HB2	2:B:32:LYS:NZ	2.17	0.59
1:A:120:LEU:HD22	1:A:121:ASP:H	1.66	0.59
1:A:242:GLN:O	1:A:244:ILE:HD12	2.02	0.59
1:A:199:ARG:HG2	1:A:199:ARG:NH1	2.12	0.59
1:A:54:ASN:ND2	1:A:56:TYR:H	2.01	0.59
1:A:238:LYS:HD2	1:A:315:HIS:CG	2.38	0.59
1:A:287:LYS:HE3	1:A:291:GLU:OE2	2.02	0.59
2:B:81:ASN:HD21	2:B:154:LYS:H	1.50	0.58
2:B:275:LYS:H	2:B:306:ASN:HD21	1.51	0.58
2:B:393:ILE:HG12	2:B:394:GLN:N	2.19	0.58
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.68	0.58
2:B:296:THR:HG22	2:B:298:GLU:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.39	0.57
2:B:80:LEU:HD22	2:B:84:THR:HG23	1.87	0.57
2:B:393:ILE:HG12	2:B:394:GLN:H	1.69	0.57
2:B:81:ASN:HD21	2:B:153:TRP:HA	1.70	0.56
2:B:12:LEU:HD23	2:B:84:THR:HG22	1.87	0.56
2:B:345:PRO:O	2:B:346:PHE:HB2	2.04	0.56
1:A:362:THR:HG22	1:A:366:LYS:HD2	1.87	0.56
1:A:195:ILE:O	1:A:199:ARG:HG3	2.06	0.56
2:B:91:GLN:C	2:B:91:GLN:HE21	2.09	0.56
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.88	0.56
2:B:184:MET:HE2	5:B:498:HOH:O	2.06	0.55
1:A:19:PRO:HG3	1:A:80:LEU:HA	1.88	0.55
1:A:312:GLU:CD	1:A:312:GLU:H	2.09	0.55
2:B:305:GLU:O	2:B:309:ILE:HG13	2.06	0.55
1:A:483:TYR:O	1:A:487:GLN:HG2	2.06	0.55
2:B:206:ARG:CZ	2:B:206:ARG:HB3	2.37	0.55
1:A:278:GLN:HG3	1:A:298:GLU:HB2	1.89	0.55
1:A:129:ALA:HA	1:A:144:TYR:O	2.06	0.55
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.88	0.55
2:B:259:LYS:NZ	2:B:425:LEU:HD11	2.23	0.54
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.38	0.54
1:A:368:LEU:HD22	1:A:423:VAL:HG11	1.90	0.54
1:A:120:LEU:HD22	1:A:121:ASP:N	2.21	0.54
2:B:282:LEU:HB3	2:B:293:ILE:HD13	1.90	0.54
2:B:344:GLU:HB2	2:B:347:LYS:HD3	1.88	0.54
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.88	0.54
1:A:92:LEU:H	1:A:92:LEU:CD2	2.17	0.54
1:A:350:LYS:HE3	1:A:378:GLU:OE2	2.08	0.53
2:B:183:TYR:CD2	2:B:380:ILE:HD13	2.43	0.53
1:A:503:LEU:CD1	1:A:533:LEU:HD12	2.35	0.53
1:A:536:VAL:HG13	1:A:542:ILE:HG13	1.89	0.53
1:A:255:ASN:HB2	1:A:289:LEU:HG	1.91	0.53
1:A:24:TRP:CD2	1:A:25:PRO:HD2	2.44	0.53
1:A:393:ILE:CB	1:A:423:VAL:HG13	2.40	0.52
2:B:253:THR:O	2:B:257:ILE:HG12	2.09	0.52
1:A:27:THR:HG21	5:A:610:HOH:O	2.09	0.52
1:A:27:THR:CG2	1:A:29:GLU:HG2	2.39	0.52
1:A:205:LEU:HD22	1:A:209:LEU:HD22	1.92	0.52
2:B:425:LEU:HD12	2:B:428:GLN:OE1	2.09	0.52
1:A:27:THR:O	1:A:31:ILE:HG13	2.10	0.52
2:B:395:LYS:O	2:B:399:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:THR:HG22	1:A:198:HIS:NE2	2.24	0.52
1:A:143:ARG:NH1	1:A:143:ARG:HG2	2.26	0.51
1:A:200:THR:O	1:A:204:GLU:HG3	2.10	0.51
1:A:278:GLN:HB3	1:A:299:ALA:HA	1.92	0.51
1:A:369:THR:O	1:A:373:GLN:HG2	2.09	0.51
2:B:65:LYS:HB2	2:B:68:SER:HB2	1.92	0.51
2:B:259:LYS:HZ3	2:B:425:LEU:HD11	1.75	0.51
1:A:27:THR:HG21	1:A:29:GLU:HG2	1.92	0.51
1:A:107:THR:HG21	1:A:202:ILE:HG13	1.91	0.51
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.76	0.51
1:A:8:VAL:O	1:A:10:VAL:HG23	2.10	0.51
1:A:542:ILE:HD11	2:B:261:VAL:HG11	1.92	0.50
1:A:500:GLN:NE2	2:B:422:LEU:HD23	2.27	0.50
1:A:90:VAL:CG2	1:A:91:GLN:H	2.13	0.50
1:A:450:THR:O	1:A:451:LYS:HB2	2.12	0.50
1:A:393:ILE:HG13	1:A:423:VAL:HG13	1.92	0.50
2:B:306:ASN:O	2:B:310:LEU:HD22	2.11	0.50
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.10	0.50
1:A:420:PRO:HA	1:A:421:PRO:C	2.32	0.49
1:A:175:ASN:HD22	1:A:201:LYS:HZ1	1.59	0.49
1:A:529:GLU:O	1:A:530:LYS:HG3	2.11	0.49
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.47	0.49
2:B:30:LYS:HE3	2:B:403:THR:HG21	1.93	0.49
2:B:394:GLN:NE2	2:B:396:GLU:HB2	2.27	0.49
1:A:207:GLN:NE2	1:A:207:GLN:HA	2.28	0.49
1:A:547:GLN:O	1:A:551:LEU:HD13	2.13	0.49
2:B:214:LEU:HD13	2:B:214:LEU:O	2.12	0.49
1:A:126:LYS:HA	1:A:145:GLN:NE2	2.28	0.49
1:A:52:PRO:HA	1:A:54:ASN:N	2.27	0.48
1:A:451:LYS:HD2	1:A:451:LYS:N	2.28	0.48
1:A:178:ILE:HG12	1:A:179:VAL:N	2.27	0.48
2:B:165:THR:HG22	5:B:459:HOH:O	2.12	0.48
2:B:167:ILE:HG12	2:B:212:TRP:CD2	2.48	0.48
2:B:296:THR:O	2:B:300:GLU:HG2	2.13	0.48
2:B:24:TRP:CZ3	2:B:399:GLU:HB3	2.48	0.48
2:B:355:ALA:O	2:B:356:ARG:HB3	2.13	0.48
1:A:178:ILE:HD13	1:A:178:ILE:C	2.34	0.48
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.49	0.48
2:B:24:TRP:N	2:B:24:TRP:CD1	2.81	0.48
1:A:52:PRO:CA	1:A:53:GLU:C	2.77	0.48
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:SER:HB2	1:A:193:LEU:CD2	2.42	0.48
2:B:376:THR:O	2:B:380:ILE:HG13	2.14	0.47
1:A:450:THR:CG2	1:A:452:LEU:HB2	2.41	0.47
2:B:394:GLN:HE21	2:B:396:GLU:HB2	1.78	0.47
1:A:517:LEU:HA	1:A:520:GLN:NE2	2.29	0.47
2:B:237:ASP:C	2:B:239:TRP:H	2.18	0.47
1:A:230:MET:HE3	5:A:620:HOH:O	2.14	0.47
1:A:393:ILE:CG1	1:A:423:VAL:HG13	2.45	0.47
2:B:154:LYS:HG2	2:B:184:MET:CE	2.45	0.47
1:A:126:LYS:HD2	5:A:652:HOH:O	2.15	0.47
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.97	0.47
2:B:169:GLU:OE1	2:B:173:LYS:HE3	2.15	0.47
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.74	0.47
2:B:58:THR:HG23	2:B:76:ASP:O	2.15	0.47
1:A:92:LEU:CD1	2:B:22:LYS:HE2	2.44	0.46
1:A:191:SER:CB	1:A:193:LEU:HD23	2.45	0.46
2:B:388:LYS:HE2	2:B:415:GLU:OE1	2.14	0.46
1:A:53:GLU:O	1:A:54:ASN:C	2.54	0.46
2:B:30:LYS:HE3	2:B:403:THR:CG2	2.44	0.46
1:A:457:TYR:HA	1:A:548:VAL:HG21	1.96	0.46
1:A:349:LEU:HD12	1:A:349:LEU:N	2.30	0.46
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.51	0.46
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.50	0.46
1:A:392:PRO:O	1:A:423:VAL:HG12	2.15	0.46
1:A:27:THR:HG22	1:A:29:GLU:N	2.29	0.46
2:B:13:LYS:HE3	2:B:16:MET:CE	2.46	0.46
1:A:92:LEU:HD12	2:B:22:LYS:HE2	1.98	0.46
2:B:398:TRP:O	2:B:402:TRP:HD1	1.99	0.46
1:A:220:LYS:HD2	1:A:220:LYS:HA	1.62	0.46
1:A:538:ALA:HA	1:A:545:ASN:HD21	1.81	0.46
2:B:80:LEU:HD13	2:B:153:TRP:CD1	2.51	0.45
2:B:239:TRP:NE1	4:B:441:SO4:O4	2.47	0.45
2:B:320:ASP:OD2	2:B:323:LYS:HD3	2.16	0.45
1:A:298:GLU:CD	1:A:298:GLU:N	2.68	0.45
1:A:406:TRP:CE3	1:A:407:GLN:NE2	2.85	0.45
1:A:345:PRO:HA	1:A:346:PHE:HA	1.53	0.45
2:B:282:LEU:HB3	2:B:293:ILE:CD1	2.45	0.45
1:A:513:SER:H	1:A:519:ASN:HD21	1.64	0.45
2:B:175:ASN:HD21	2:B:201:LYS:HZ2	1.65	0.45
1:A:494:ASN:HB3	2:B:289:LEU:HD12	1.99	0.45
1:A:54:ASN:HD22	1:A:54:ASN:C	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:LEU:HD22	2:B:422:LEU:N	2.32	0.45
1:A:524:GLN:NE2	5:A:589:HOH:O	2.50	0.45
2:B:254:VAL:O	2:B:258:GLN:HG3	2.16	0.45
1:A:358:ARG:NH1	2:B:394:GLN:HG3	2.33	0.44
2:B:278:GLN:NE2	2:B:298:GLU:HB3	2.32	0.44
2:B:214:LEU:HD13	2:B:214:LEU:C	2.37	0.44
1:A:175:ASN:ND2	1:A:201:LYS:HZ1	2.14	0.44
1:A:169:GLU:CB	1:A:170:PRO:HD3	2.46	0.44
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.52	0.44
1:A:332:GLN:NE2	1:A:338:THR:HG21	2.33	0.44
1:A:54:ASN:HD22	1:A:56:TYR:H	1.66	0.44
2:B:64:LYS:O	2:B:65:LYS:C	2.56	0.44
1:A:536:VAL:CG1	1:A:542:ILE:HG13	2.46	0.44
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.81	0.44
1:A:100:LEU:O	1:A:318:TYR:HB3	2.18	0.44
1:A:60:VAL:HG11	1:A:130:PHE:CD2	2.53	0.44
1:A:411:ILE:HG13	1:A:414:TRP:CD1	2.53	0.44
3:A:561:65B:N12	3:A:561:65B:H26	2.33	0.43
2:B:368:LEU:O	2:B:372:VAL:HG23	2.19	0.43
2:B:32:LYS:HZ3	2:B:32:LYS:HB2	1.83	0.43
1:A:538:ALA:HA	1:A:545:ASN:ND2	2.33	0.43
1:A:126:LYS:HG2	1:A:127:TYR:N	2.34	0.42
2:B:386:THR:CG2	2:B:412:PRO:HB3	2.49	0.42
1:A:175:ASN:ND2	1:A:201:LYS:HZ3	2.18	0.42
1:A:178:ILE:HD11	1:A:180:ILE:HG13	2.00	0.42
1:A:279:LEU:O	1:A:282:LEU:HB2	2.18	0.42
2:B:303:LEU:HD23	2:B:303:LEU:N	2.35	0.42
1:A:27:THR:CG2	1:A:28:GLU:N	2.82	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.42
1:A:211:ARG:NH2	5:A:572:HOH:O	2.52	0.42
2:B:214:LEU:HD13	2:B:215:THR:O	2.20	0.42
1:A:96:HIS:CE1	1:A:350:LYS:HD2	2.55	0.42
1:A:242:GLN:HB2	1:A:243:PRO:HD2	2.02	0.42
1:A:77:PHE:O	1:A:78:ARG:C	2.58	0.42
2:B:405:TYR:O	2:B:407:GLN:HG3	2.20	0.42
1:A:188:TYR:HB3	3:A:561:65B:C3	2.49	0.41
1:A:413:GLU:HA	5:A:605:HOH:O	2.20	0.41
1:A:508:ALA:O	1:A:509:GLN:HB3	2.20	0.41
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.49	0.41
2:B:422:LEU:HB3	2:B:426:TRP:CH2	2.55	0.41
2:B:266:TRP:CH2	2:B:427:TYR:CZ	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:373:GLN:HE22	2:B:407:GLN:N	2.15	0.41
2:B:30:LYS:HD2	2:B:62:ALA:HB3	2.02	0.41
2:B:237:ASP:C	2:B:239:TRP:N	2.74	0.41
2:B:105:SER:O	2:B:190:GLY:HA2	2.20	0.41
2:B:244:ILE:HG12	2:B:266:TRP:HZ3	1.85	0.41
1:A:3:SER:OG	1:A:5:ILE:HG22	2.20	0.41
2:B:24:TRP:H	2:B:24:TRP:HD1	1.69	0.41
1:A:548:VAL:O	1:A:552:VAL:HG22	2.21	0.41
2:B:69:THR:C	2:B:70:LYS:HG3	2.40	0.41
1:A:473:THR:O	1:A:477:THR:HG23	2.21	0.41
1:A:63:ILE:HD11	1:A:74:LEU:HD12	2.03	0.41
1:A:509:GLN:N	1:A:510:PRO:CD	2.83	0.41
1:A:139:THR:HB	1:A:140:PRO:HD2	2.02	0.40
1:A:388:LYS:HE2	1:A:388:LYS:HB3	1.83	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	546/560 (98%)	511 (94%)	29 (5%)	6 (1%)	17 18
2	B	393/440 (89%)	378 (96%)	14 (4%)	1 (0%)	46 57
All	All	939/1000 (94%)	889 (95%)	43 (5%)	7 (1%)	26 31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	90	VAL
1	A	218	ASP
2	B	250	ASP

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Mol	Chain	Res	Type
1	A	543	GLY
1	A	78	ARG
1	A	509	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	492/500 (98%)	457 (93%)	35 (7%)	18	23
2	B	366/400 (92%)	344 (94%)	22 (6%)	24	31
All	All	858/900 (95%)	801 (93%)	57 (7%)	21	27

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	54	ASN
1	A	67	ASP
1	A	92	LEU
1	A	94	ILE
1	A	107	THR
1	A	120	LEU
1	A	126	LYS
1	A	178	ILE
1	A	194	GLU
1	A	205	LEU
1	A	209	LEU
1	A	218	ASP
1	A	219	LYS
1	A	220	LYS
1	A	264	LEU
1	A	275	LYS
1	A	282	LEU
1	A	283	LEU
1	A	301	LEU

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Mol	Chain	Res	Type
1	A	303	LEU
1	A	310	LEU
1	A	312	GLU
1	A	347	LYS
1	A	350	LYS
1	A	402	TRP
1	A	423	VAL
1	A	448	ARG
1	A	449	GLU
1	A	474	ASN
1	A	479	LEU
1	A	517	LEU
1	A	523	GLU
1	A	529	GLU
1	A	533	LEU
2	B	30	LYS
2	B	48	SER
2	B	80	LEU
2	B	91	GLN
2	B	92	LEU
2	B	113	ASP
2	B	165	THR
2	B	184	MET
2	B	194	GLU
2	B	205	LEU
2	B	209	LEU
2	B	234	LEU
2	B	250	ASP
2	B	260	LEU
2	B	295	LEU
2	B	310	LEU
2	B	323	LYS
2	B	353	LYS
2	B	368	LEU
2	B	369	THR
2	B	374	LYS
2	B	429	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	57	ASN
1	A	91	GLN
1	A	145	GLN
1	A	174	GLN
1	A	175	ASN
1	A	207	GLN
1	A	258	GLN
1	A	269	GLN
1	A	306	ASN
1	A	332	GLN
1	A	407	GLN
1	A	500	GLN
1	A	509	GLN
1	A	519	ASN
1	A	520	GLN
1	A	545	ASN
2	B	81	ASN
2	B	85	GLN
2	B	91	GLN
2	B	147	ASN
2	B	151	GLN
2	B	175	ASN
2	B	208	HIS
2	B	255	ASN
2	B	258	GLN
2	B	278	GLN
2	B	306	ASN
2	B	336	GLN
2	B	348	ASN
2	B	367	GLN
2	B	373	GLN
2	B	394	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
3	65B	A	561	-	30,30,30	2.59	15 (50%)	38,42,42	1.60	5 (13%)
4	SO4	A	562	-	4,4,4	0.17	0	6,6,6	0.17	0
4	SO4	A	563	-	4,4,4	0.21	0	6,6,6	0.14	0
4	SO4	A	564	-	4,4,4	0.20	0	6,6,6	0.12	0
4	SO4	A	565	-	4,4,4	0.22	0	6,6,6	0.11	0
4	SO4	B	441	-	4,4,4	0.55	0	6,6,6	0.29	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
3	65B	A	561	-	-	0/12/12/12	0/3/3/3
4	SO4	A	562	-	-	0/0/0/0	0/0/0/0
4	SO4	A	563	-	-	0/0/0/0	0/0/0/0
4	SO4	A	564	-	-	0/0/0/0	0/0/0/0
4	SO4	A	565	-	-	0/0/0/0	0/0/0/0
4	SO4	B	441	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	65B	C5-C4	2.07	1.43	1.39
3	A	561	65B	C6'-C6	2.07	1.55	1.51
3	A	561	65B	C11-N16	2.19	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	65B	C23-C24	2.27	1.44	1.39
3	A	561	65B	C25-C24	2.27	1.44	1.39
3	A	561	65B	C23-C22	2.28	1.42	1.38
3	A	561	65B	C22-C21	2.66	1.43	1.39
3	A	561	65B	C3-C2	2.77	1.43	1.39
3	A	561	65B	C5-C6	2.92	1.43	1.39
3	A	561	65B	C26-C25	3.33	1.44	1.38
3	A	561	65B	C1-C2	3.56	1.46	1.40
3	A	561	65B	C1-C6	3.69	1.46	1.40
3	A	561	65B	C15-N16	5.04	1.42	1.35
3	A	561	65B	C26-C21	5.35	1.48	1.39
3	A	561	65B	C13-N12	6.13	1.41	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	561	65B	N16-C11-N12	-5.31	118.06	126.22
3	A	561	65B	C14-C13-N12	-3.24	120.53	124.00
3	A	561	65B	C14-C15-N18	-2.01	121.14	122.87
3	A	561	65B	C11-N16-C15	2.19	120.74	116.91
3	A	561	65B	C11-N12-C13	4.78	122.27	115.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	561	65B	2	0
4	B	441	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

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	550/560 (98%)	0.30	24 (4%)	38	47	30, 50, 90, 122	0
2	B	401/440 (91%)	0.34	26 (6%)	22	30	27, 49, 89, 104	0
All	All	951/1000 (95%)	0.32	50 (5%)	30	39	27, 50, 89, 122	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	ASP	4.9
2	B	87	PHE	3.7
1	A	220	LYS	3.6
1	A	286	THR	3.4
2	B	277	ARG	3.3
2	B	295	LEU	3.3
2	B	90	VAL	3.1
2	B	14	PRO	3.1
2	B	92	LEU	3.0
2	B	10	VAL	3.0
2	B	15	GLY	3.0
1	A	219	LYS	2.9
2	B	362	THR	2.9
2	B	276	VAL	2.9
2	B	283	LEU	2.9
1	A	66	LYS	2.7
2	B	284	ARG	2.7
1	A	67	ASP	2.7
1	A	426	TRP	2.6
2	B	298	GLU	2.6
2	B	355	ALA	2.6
2	B	24	TRP	2.5
1	A	223	LYS	2.5
1	A	24	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	552	VAL	2.5
1	A	70	LYS	2.5
1	A	547	GLN	2.5
2	B	281	LYS	2.5
1	A	53	GLU	2.4
1	A	406	TRP	2.4
2	B	346	PHE	2.4
2	B	252	TRP	2.3
2	B	266	TRP	2.3
1	A	425	LEU	2.3
2	B	12	LEU	2.3
1	A	402	TRP	2.3
2	B	70	LYS	2.3
1	A	357	MET	2.3
2	B	238	LYS	2.3
2	B	279	LEU	2.2
1	A	63	ILE	2.2
2	B	88	TRP	2.2
2	B	278	GLN	2.2
1	A	194	GLU	2.2
1	A	199	ARG	2.2
1	A	104	LYS	2.1
1	A	207	GLN	2.1
2	B	116	PHE	2.0
1	A	22	LYS	2.0
1	A	454	LYS	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
4	SO4	A	564	5/5	0.76	0.20	2.37	138,138,139,139	0
4	SO4	B	441	5/5	0.94	0.23	0.89	96,96,97,97	0
3	65B	A	561	28/28	0.93	0.15	0.70	35,38,42,70	0
4	SO4	A	562	5/5	0.97	0.13	0.43	71,72,73,74	0
4	SO4	A	563	5/5	0.95	0.14	-0.27	73,75,76,76	0
4	SO4	A	565	5/5	0.91	0.15	-	105,106,106,106	0

6.5 Other polymers (i)

There are no such residues in this entry.