Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:50 AM GMT

PDB ID	:	3JV6
Title	:	Crystal structure of the dimerization domains p52 and RelB
Authors	:	Vu, D.; Huang, D.B.; Ghosh, G.
Deposited on	:	2009-09-15
Resolution	:	2.78 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:

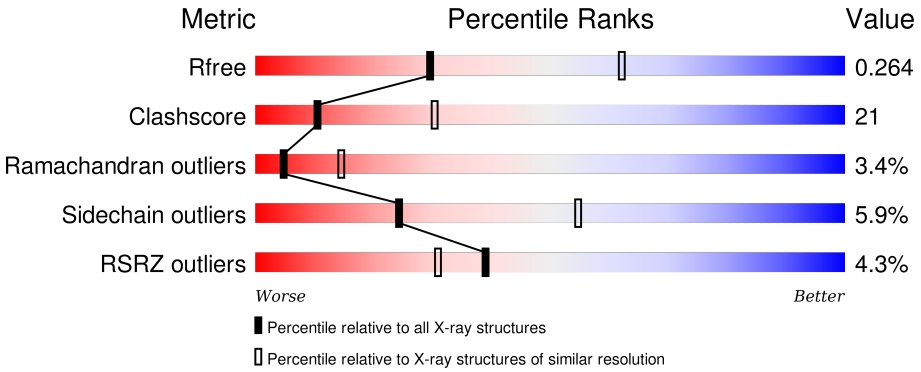
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.78 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	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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	101	% 61% 34% 5%
1	C	101	52% 43% 5%
1	E	101	% 55% 41% .
2	B	107	3% 58% 32% 10%
2	D	107	10% 64% 31% . .

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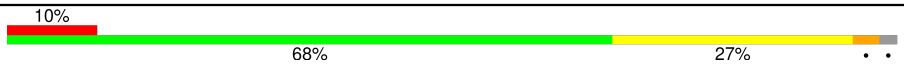
Mol	Chain	Length	Quality of chain
2	F	107	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	601	-	-	-	X
3	SO4	D	603	-	-	-	X
3	SO4	D	608	-	X	-	-
3	SO4	F	602	-	-	-	X
3	SO4	F	609	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5191 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 Transcription factor RelB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	0	0	0
			800	507	132	157	4			
1	C	101	Total	C	N	O	S	0	0	0
			800	507	132	157	4			
1	E	101	Total	C	N	O	S	0	0	0
			800	507	132	157	4			

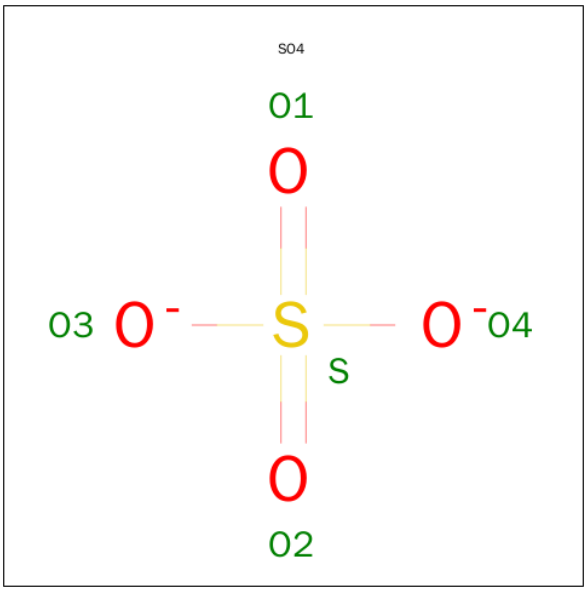
- Molecule 2 is a protein called Nuclear factor NF-kappa-B p100 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	107	Total	C	N	O	S	0	0	0
			875	555	150	167	3			
2	D	106	Total	C	N	O	S	0	0	0
			867	551	149	164	3			
2	F	105	Total	C	N	O	S	0	0	0
			858	546	148	161	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	328	VAL	LEU	CONFLICT	UNP Q9WTK5
D	328	VAL	LEU	CONFLICT	UNP Q9WTK5
F	328	VAL	LEU	CONFLICT	UNP Q9WTK5

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	29	Total O 29 29	0	0
4	B	28	Total O 28 28	0	0
4	C	28	Total O 28 28	0	0

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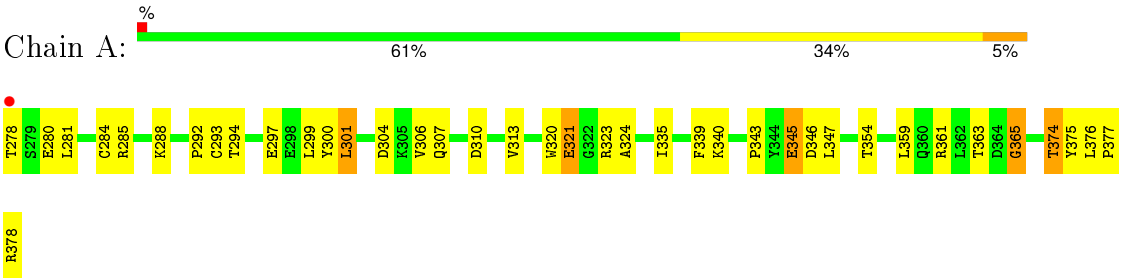
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	19	Total O 19 19	0	0
4	E	21	Total O 21 21	0	0
4	F	21	Total O 21 21	0	0

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.

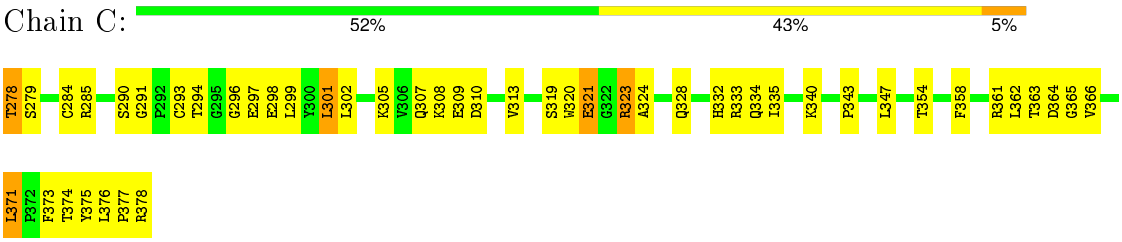
- Molecule 1: Transcription factor RelB

Chain A:



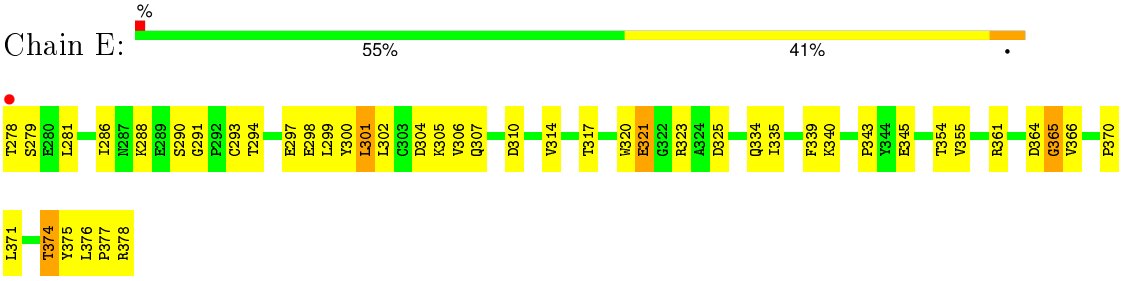
- Molecule 1: Transcription factor RelB

Chain C:



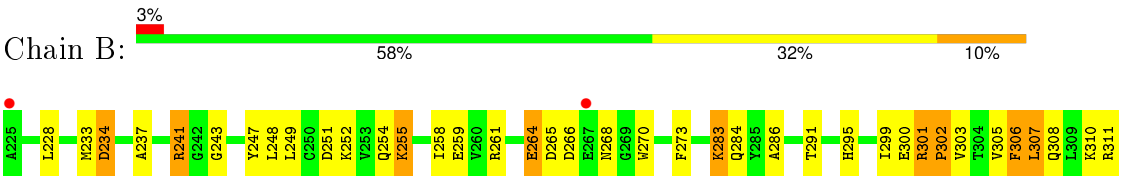
- Molecule 1: Transcription factor RelB

Chain E:



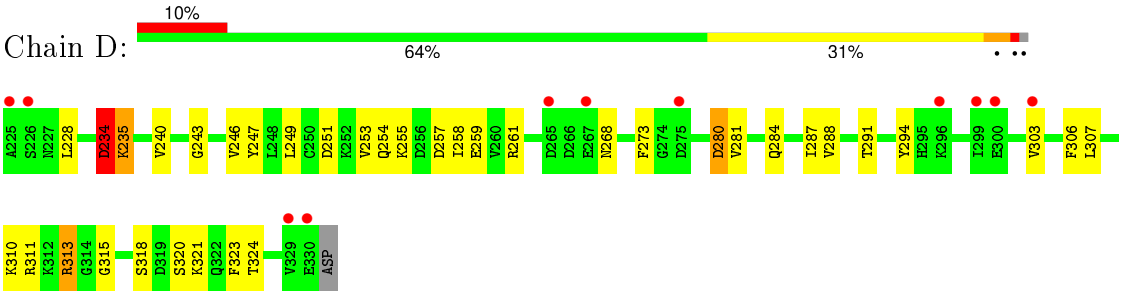
- Molecule 2: Nuclear factor NF-kappa-B p100 subunit

Chain B:



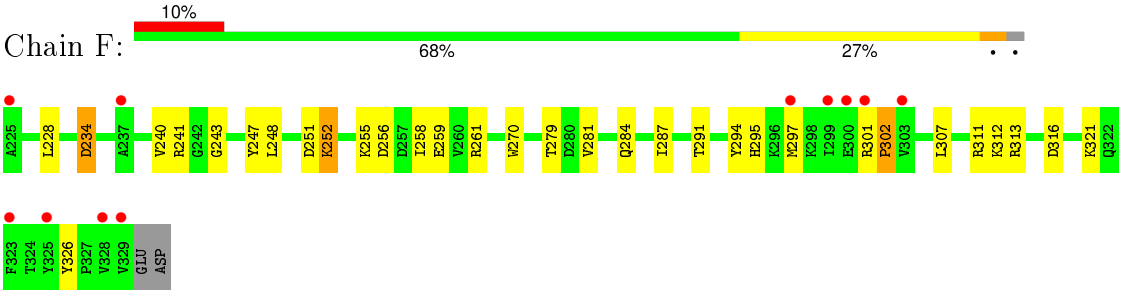
• Molecule 2: Nuclear factor NF-kappa-B p100 subunit

Chain D:



• Molecule 2: Nuclear factor NF-kappa-B p100 subunit

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	126.33Å 141.14Å 168.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.63 – 2.78 39.09 – 2.78	Depositor EDS
% Data completeness (in resolution range)	70.3 (29.63-2.78) 80.3 (39.09-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.248 0.226 , 0.264	Depositor DCC
R_{free} test set	1676 reflections (5.75%)	DCC
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	1.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	4 of 33723 reflections (0.012%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5191	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: 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	0.37	0/817	0.67	0/1111
1	C	0.35	0/817	0.67	0/1111
1	E	0.37	0/817	0.69	0/1111
2	B	0.38	0/895	0.67	0/1206
2	D	0.35	0/887	0.63	0/1195
2	F	0.37	0/878	0.65	0/1183
All	All	0.37	0/5111	0.66	0/6917

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	800	0	785	33	0
1	C	800	0	785	48	0
1	E	800	0	785	46	0
2	B	875	0	850	38	0
2	D	867	0	846	29	0
2	F	858	0	840	24	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	1	0
3	C	5	0	0	1	0
3	D	10	0	0	0	0
3	E	5	0	0	0	0
3	F	10	0	0	0	0
4	A	29	0	0	0	0
4	B	28	0	0	2	0
4	C	28	0	0	0	0
4	D	19	0	0	1	0
4	E	21	0	0	1	0
4	F	21	0	0	0	0
All	All	5191	0	4891	213	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 21.

All (213) 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:354:THR:HG22	1:A:374:THR:HB	1.44	0.99
2:B:301:ARG:HH11	2:B:301:ARG:HB3	1.26	0.98
1:C:378:ARG:HB3	1:C:378:ARG:NH1	1.82	0.93
1:C:378:ARG:HB3	1:C:378:ARG:HH11	1.33	0.92
2:D:234:ASP:HB2	2:D:247:TYR:H	1.39	0.88
1:E:323:ARG:HG3	1:E:323:ARG:HH21	1.46	0.80
1:A:354:THR:HG22	1:A:374:THR:CB	2.14	0.78
1:A:377:PRO:O	1:A:378:ARG:HB2	1.82	0.78
2:B:234:ASP:HB2	2:B:247:TYR:HB2	1.69	0.74
2:F:228:LEU:HD21	2:F:311:ARG:NH1	2.02	0.74
2:F:234:ASP:HB2	2:F:247:TYR:HB2	1.69	0.73
1:E:299:LEU:HB2	1:E:339:PHE:CE1	2.24	0.71
1:E:378:ARG:HG2	1:E:378:ARG:HH11	1.56	0.70
1:C:290:SER:HB2	1:C:376:LEU:HD21	1.71	0.70
1:E:377:PRO:O	1:E:378:ARG:HB3	1.90	0.70
1:C:310:ASP:CG	1:C:363:THR:HG23	2.13	0.68
1:E:323:ARG:HG3	1:E:323:ARG:NH2	2.10	0.67
1:E:354:THR:HG22	1:E:374:THR:CG2	2.23	0.67
1:C:320:TRP:CG	1:C:321:GLU:N	2.61	0.67
1:C:354:THR:HB	1:C:374:THR:HG22	1.77	0.66
1:C:307:GLN:HE21	1:C:307:GLN:HA	1.59	0.66
1:C:310:ASP:OD1	1:C:363:THR:HG23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:THR:HG22	1:E:374:THR:HB	1.78	0.66
1:C:307:GLN:NE2	1:C:307:GLN:HA	2.11	0.66
1:E:290:SER:HB2	1:E:376:LEU:HD11	1.78	0.66
2:F:234:ASP:CB	2:F:247:TYR:H	2.08	0.65
1:E:297:GLU:O	1:E:340:LYS:HA	1.97	0.64
2:B:259:GLU:OE1	2:B:273:PHE:HE1	1.81	0.63
1:A:310:ASP:OD1	1:A:363:THR:HG23	1.99	0.63
1:E:294:THR:O	1:E:343:PRO:HB3	1.98	0.63
1:A:320:TRP:CG	1:A:321:GLU:N	2.67	0.63
2:B:259:GLU:OE2	2:B:312:LYS:HG2	1.99	0.63
1:C:301:LEU:HD12	1:C:301:LEU:O	1.99	0.62
2:D:234:ASP:HB3	2:D:235:LYS:HD2	1.81	0.62
1:E:320:TRP:CG	1:E:321:GLU:N	2.68	0.61
1:A:301:LEU:O	1:A:301:LEU:HD12	1.99	0.61
2:B:306:PHE:N	2:B:306:PHE:CD2	2.68	0.61
1:A:354:THR:HA	1:A:374:THR:HA	1.82	0.61
1:E:281:LEU:HD12	1:E:361:ARG:HH21	1.66	0.61
1:A:354:THR:CG2	1:A:374:THR:HB	2.27	0.60
1:C:354:THR:CB	1:C:374:THR:HG22	2.31	0.60
1:E:291:GLY:H	1:E:376:LEU:HD13	1.67	0.60
1:E:361:ARG:O	1:E:365:GLY:HA2	2.02	0.59
1:C:313:VAL:HB	1:C:324:ALA:HB3	1.84	0.59
2:B:299:ILE:HD12	2:B:303:VAL:HG23	1.84	0.59
1:C:297:GLU:O	1:C:340:LYS:HA	2.03	0.59
2:B:306:PHE:N	2:B:306:PHE:HD2	2.00	0.59
2:B:301:ARG:NH1	2:B:301:ARG:HB3	2.08	0.59
1:A:293:CYS:HA	1:A:375:TYR:CD2	2.38	0.58
1:C:377:PRO:O	1:C:378:ARG:HB2	2.02	0.58
2:B:234:ASP:CB	2:B:247:TYR:H	2.17	0.58
1:A:354:THR:HG22	1:A:374:THR:CG2	2.33	0.58
1:A:307:GLN:HA	1:A:307:GLN:HE21	1.69	0.58
2:D:310:LYS:HE3	2:D:315:GLY:O	2.04	0.58
1:C:296:GLY:O	1:C:340:LYS:HD3	2.03	0.57
2:F:270:TRP:CD1	2:F:295:HIS:HB3	2.39	0.57
1:A:301:LEU:HD12	1:A:301:LEU:C	2.24	0.57
1:A:301:LEU:HD23	1:A:339:PHE:HE2	1.69	0.57
1:A:297:GLU:O	1:A:340:LYS:HA	2.04	0.57
1:C:364:ASP:CG	1:C:366:VAL:HG23	2.24	0.57
1:A:292:PRO:HD2	1:A:297:GLU:OE2	2.05	0.56
1:A:307:GLN:HA	1:A:307:GLN:NE2	2.20	0.56
2:F:256:ASP:O	2:F:312:LYS:HE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:GLU:OE1	2:B:273:PHE:CE1	2.59	0.56
1:C:354:THR:HB	1:C:374:THR:CG2	2.36	0.55
2:D:240:VAL:HG23	2:D:294:TYR:HB3	1.89	0.55
1:C:294:THR:O	1:C:343:PRO:HB3	2.07	0.55
1:E:354:THR:HG22	1:E:374:THR:CB	2.36	0.55
1:C:298:GLU:O	1:C:299:LEU:HD23	2.07	0.55
1:A:300:TYR:CE2	2:B:234:ASP:HA	2.42	0.55
1:C:309:GLU:HA	1:C:328:GLN:NE2	2.20	0.55
1:C:320:TRP:O	1:C:321:GLU:HB2	2.07	0.55
1:E:370:PRO:C	1:E:371:LEU:HD12	2.27	0.54
1:C:308:LYS:HD2	1:C:328:GLN:HB3	1.88	0.54
1:C:293:CYS:HA	1:C:375:TYR:CD2	2.43	0.54
2:F:261:ARG:O	2:F:307:LEU:HA	2.07	0.54
1:E:307:GLN:HA	1:E:307:GLN:HE21	1.72	0.54
1:E:302:LEU:HD13	2:F:247:TYR:HE2	1.73	0.54
2:F:240:VAL:HG11	2:F:297:MET:HA	1.90	0.54
1:C:335:ILE:HD12	1:C:335:ILE:C	2.26	0.54
1:E:317:THR:CG2	1:E:355:VAL:HG12	2.38	0.54
1:E:370:PRO:O	1:E:371:LEU:HD12	2.08	0.53
1:C:321:GLU:HG2	1:C:323:ARG:HH21	1.73	0.53
2:B:258:ILE:HG13	2:B:259:GLU:N	2.24	0.53
2:D:281:VAL:HG22	2:D:287:ILE:HG12	1.89	0.53
1:C:291:GLY:H	1:C:376:LEU:CD2	2.21	0.53
1:E:354:THR:HA	1:E:374:THR:HA	1.90	0.53
1:E:293:CYS:HA	1:E:375:TYR:CD2	2.45	0.52
2:D:234:ASP:CB	2:D:247:TYR:H	2.17	0.52
1:E:317:THR:HG22	1:E:355:VAL:HG12	1.92	0.52
2:B:311:ARG:HD3	4:B:482:HOH:O	2.09	0.52
1:E:314:VAL:HG22	1:E:323:ARG:HG2	1.90	0.52
1:E:378:ARG:HG2	1:E:378:ARG:NH1	2.22	0.52
2:D:251:ASP:O	2:D:253:VAL:HG13	2.10	0.52
1:A:313:VAL:HB	1:A:324:ALA:HB3	1.92	0.52
2:D:307:LEU:HD23	2:D:323:PHE:HB2	1.92	0.52
2:F:240:VAL:HG12	2:F:297:MET:SD	2.51	0.51
1:E:299:LEU:HD12	1:E:339:PHE:HE1	1.76	0.51
2:D:235:LYS:HD3	2:D:246:VAL:HG22	1.91	0.51
1:E:307:GLN:HA	1:E:307:GLN:NE2	2.26	0.51
1:E:278:THR:HG23	1:E:279:SER:H	1.76	0.51
2:B:261:ARG:O	2:B:307:LEU:HA	2.11	0.50
2:B:234:ASP:HB3	2:B:247:TYR:H	1.77	0.50
1:A:294:THR:O	1:A:343:PRO:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:HIS:CE1	1:C:333:ARG:HD3	2.47	0.50
1:E:300:TYR:CE1	2:F:234:ASP:HA	2.45	0.50
2:D:234:ASP:HB2	2:D:247:TYR:N	2.18	0.50
1:C:305:LYS:HA	1:C:334:GLN:O	2.12	0.50
2:B:270:TRP:CD1	2:B:295:HIS:HB3	2.47	0.49
2:B:243:GLY:N	2:B:291:THR:O	2.38	0.49
2:B:301:ARG:N	2:B:301:ARG:HD2	2.27	0.49
2:F:307:LEU:HD21	2:F:321:LYS:HB2	1.93	0.49
1:C:321:GLU:HG2	1:C:323:ARG:NH2	2.27	0.49
1:A:335:ILE:HD12	1:A:335:ILE:C	2.33	0.48
1:C:376:LEU:N	1:C:376:LEU:HD22	2.28	0.48
2:B:305:VAL:C	2:B:306:PHE:HD2	2.17	0.48
2:F:258:ILE:HG13	2:F:259:GLU:N	2.28	0.48
1:E:298:GLU:O	1:E:299:LEU:HD23	2.13	0.48
1:E:320:TRP:CD1	1:E:345:GLU:HB2	2.48	0.48
1:A:345:GLU:HG2	1:A:346:ASP:N	2.28	0.48
2:B:299:ILE:CD1	2:B:303:VAL:HG23	2.43	0.48
2:F:302:PRO:HG3	2:F:326:TYR:HD1	1.78	0.47
2:B:301:ARG:CB	2:B:301:ARG:HH11	2.12	0.47
1:A:284:CYS:O	1:A:285:ARG:HB3	2.14	0.47
1:E:304:ASP:O	1:E:306:VAL:HG13	2.15	0.47
1:C:361:ARG:O	1:C:365:GLY:HA2	2.15	0.47
1:A:281:LEU:HD22	1:A:359:LEU:HB2	1.96	0.47
2:D:228:LEU:CB	2:D:318:SER:HB3	2.45	0.47
2:B:264:GLU:HG2	2:B:270:TRP:HE3	1.80	0.47
2:B:308:GLN:HB3	2:B:320:SER:HB3	1.97	0.47
2:B:258:ILE:HD12	2:B:310:LYS:O	2.15	0.46
1:C:333:ARG:HD2	3:C:605:SO4:O4	2.15	0.46
2:B:330:GLU:O	2:B:331:ASP:HB2	2.15	0.46
1:C:291:GLY:H	1:C:376:LEU:HD23	1.80	0.46
1:A:301:LEU:HD23	1:A:339:PHE:CE2	2.49	0.46
2:D:261:ARG:O	2:D:307:LEU:HA	2.16	0.46
1:C:307:GLN:HE21	1:C:307:GLN:CA	2.22	0.46
1:E:320:TRP:O	1:E:321:GLU:HB2	2.16	0.46
1:A:293:CYS:HA	1:A:375:TYR:HD2	1.79	0.46
2:F:248:LEU:HD23	2:F:248:LEU:C	2.35	0.46
2:D:235:LYS:HD2	2:D:235:LYS:N	2.30	0.46
2:D:243:GLY:N	2:D:291:THR:O	2.48	0.46
2:D:306:PHE:HA	2:D:321:LYS:O	2.15	0.46
2:B:233:MET:HE1	2:B:307:LEU:HD11	1.97	0.46
1:E:364:ASP:CG	1:E:366:VAL:HG23	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:CYS:O	1:C:285:ARG:HB3	2.16	0.46
1:C:301:LEU:C	1:C:301:LEU:HD12	2.35	0.46
2:B:300:GLU:HA	2:B:300:GLU:OE1	2.16	0.46
1:C:302:LEU:CD2	2:D:247:TYR:CE2	2.99	0.46
1:E:375:TYR:C	1:E:376:LEU:HD12	2.36	0.46
1:A:307:GLN:CA	1:A:307:GLN:HE21	2.26	0.45
2:F:241:ARG:HG3	2:F:297:MET:CE	2.47	0.45
2:D:254:GLN:HB3	4:D:440:HOH:O	2.17	0.45
2:F:234:ASP:HB2	2:F:247:TYR:H	1.79	0.45
1:C:354:THR:HA	1:C:374:THR:HA	1.98	0.45
1:E:301:LEU:HD23	1:E:301:LEU:C	2.38	0.45
2:B:255:LYS:HD2	3:B:607:SO4:O1	2.17	0.45
1:C:294:THR:HA	1:C:347:LEU:HD22	1.99	0.44
2:F:313:ARG:HH21	2:F:313:ARG:HG2	1.82	0.44
1:A:304:ASP:O	1:A:306:VAL:HG13	2.16	0.44
2:D:258:ILE:HG13	2:D:259:GLU:N	2.31	0.44
1:C:332:HIS:CD2	2:D:249:LEU:HB3	2.52	0.44
1:A:288:LYS:HB2	1:A:299:LEU:HD22	1.98	0.44
1:C:291:GLY:N	1:C:376:LEU:HD23	2.33	0.44
2:B:241:ARG:HB2	2:B:241:ARG:HH11	1.82	0.44
2:B:264:GLU:OE2	2:B:295:HIS:HE1	2.00	0.44
1:E:286:ILE:HG22	1:E:288:LYS:O	2.18	0.44
2:D:253:VAL:HG22	2:D:284:GLN:O	2.18	0.44
1:E:301:LEU:HD23	1:E:301:LEU:O	2.18	0.44
2:F:252:LYS:HE3	2:F:284:GLN:NE2	2.33	0.44
1:E:361:ARG:HB2	1:E:361:ARG:HE	1.58	0.43
2:D:280:ASP:HB3	2:D:288:VAL:O	2.18	0.43
2:F:281:VAL:HG22	2:F:287:ILE:HG12	2.00	0.43
1:C:291:GLY:O	1:C:375:TYR:HA	2.18	0.43
2:B:328:VAL:O	2:B:328:VAL:HG13	2.18	0.43
2:B:302:PRO:HB2	4:B:507:HOH:O	2.19	0.43
1:C:278:THR:HG23	1:C:279:SER:H	1.83	0.43
2:B:249:LEU:HD23	2:B:286:ALA:HB2	2.01	0.43
2:F:240:VAL:HG13	2:F:294:TYR:HB3	2.01	0.42
1:A:320:TRP:O	1:A:321:GLU:HB2	2.19	0.42
1:E:335:ILE:HD12	1:E:335:ILE:C	2.40	0.42
2:B:248:LEU:HD23	2:B:248:LEU:C	2.40	0.42
2:D:261:ARG:HD2	2:D:273:PHE:HE1	1.85	0.42
2:B:237:ALA:HA	2:B:324:THR:O	2.20	0.42
2:B:266:ASP:OD1	2:B:268:ASN:HB3	2.20	0.42
1:C:371:LEU:HA	1:C:371:LEU:HD12	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:ARG:NH2	1:E:323:ARG:CG	2.81	0.41
1:C:293:CYS:HA	1:C:375:TYR:HD2	1.85	0.41
1:A:294:THR:HA	1:A:347:LEU:HD22	2.01	0.41
2:B:228:LEU:HD21	2:B:311:ARG:CZ	2.51	0.41
2:D:234:ASP:OD1	2:D:247:TYR:HB2	2.21	0.41
1:E:310:ASP:OD2	1:E:361:ARG:CG	2.67	0.41
1:E:323:ARG:HD3	4:E:449:HOH:O	2.20	0.41
1:E:302:LEU:N	1:E:302:LEU:HD12	2.36	0.41
1:C:299:LEU:HD11	1:C:373:PHE:CE2	2.56	0.41
2:D:303:VAL:O	2:D:324:THR:HG23	2.21	0.41
1:A:361:ARG:O	1:A:365:GLY:HA2	2.20	0.41
2:F:243:GLY:N	2:F:291:THR:O	2.44	0.41
1:C:378:ARG:CB	1:C:378:ARG:HH11	2.19	0.41
2:F:234:ASP:HB3	2:F:247:TYR:H	1.81	0.41
2:F:307:LEU:CD2	2:F:321:LYS:HB2	2.51	0.41
1:E:286:ILE:HG22	1:E:288:LYS:H	1.84	0.41
2:D:235:LYS:HD2	2:D:235:LYS:H	1.85	0.41
1:A:378:ARG:NH1	1:A:378:ARG:HG2	2.36	0.41
2:D:257:ASP:OD2	2:D:311:ARG:HB2	2.21	0.41
2:F:234:ASP:HB2	2:F:247:TYR:CB	2.44	0.41
2:D:228:LEU:HB3	2:D:318:SER:HB3	2.03	0.41
1:C:375:TYR:C	1:C:376:LEU:HD22	2.41	0.40
2:B:283:LYS:O	2:B:284:GLN:HB2	2.22	0.40
2:D:306:PHE:HB3	2:D:320:SER:HB2	2.02	0.40
1:A:307:GLN:CA	1:A:307:GLN:NE2	2.84	0.40
2:D:291:THR:HG21	2:D:323:PHE:CZ	2.56	0.40
1:E:305:LYS:HA	1:E:334:GLN:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	99/101 (98%)	86 (87%)	11 (11%)	2 (2%)	9 28
1	C	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	19 50
1	E	99/101 (98%)	85 (86%)	12 (12%)	2 (2%)	9 28
2	B	105/107 (98%)	90 (86%)	7 (7%)	8 (8%)	1 2
2	D	104/107 (97%)	92 (88%)	8 (8%)	4 (4%)	4 12
2	F	103/107 (96%)	92 (89%)	7 (7%)	4 (4%)	4 11
All	All	609/624 (98%)	534 (88%)	54 (9%)	21 (3%)	5 14

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	321	GLU
2	D	280	ASP
1	E	321	GLU
1	A	321	GLU
1	A	365	GLY
2	B	234	ASP
2	B	255	LYS
2	B	330	GLU
2	D	234	ASP
2	F	234	ASP
2	F	255	LYS
2	B	252	LYS
2	B	265	ASP
2	B	283	LYS
2	D	255	LYS
2	F	252	LYS
2	B	302	PRO
2	D	313	ARG
1	E	365	GLY
2	F	302	PRO
2	B	328	VAL

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	92/92 (100%)	85 (92%)	7 (8%)	16 40
1	C	92/92 (100%)	85 (92%)	7 (8%)	16 40
1	E	92/92 (100%)	89 (97%)	3 (3%)	45 78
2	B	96/96 (100%)	88 (92%)	8 (8%)	14 36
2	D	95/96 (99%)	91 (96%)	4 (4%)	36 70
2	F	94/96 (98%)	90 (96%)	4 (4%)	35 69
All	All	561/564 (100%)	528 (94%)	33 (6%)	24 55

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	THR
1	A	280	GLU
1	A	301	LEU
1	A	323	ARG
1	A	345	GLU
1	A	374	THR
1	A	376	LEU
2	B	241	ARG
2	B	251	ASP
2	B	254	GLN
2	B	264	GLU
2	B	301	ARG
2	B	306	PHE
2	B	307	LEU
2	B	316	ASP
1	C	278	THR
1	C	301	LEU
1	C	319	SER
1	C	323	ARG
1	C	358	PHE
1	C	362	LEU
1	C	371	LEU
2	D	234	ASP
2	D	235	LYS
2	D	268	ASN
2	D	313	ARG
1	E	301	LEU
1	E	325	ASP
1	E	374	THR
2	F	251	ASP

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Mol	Chain	Res	Type
2	F	279	THR
2	F	301	ARG
2	F	316	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	GLN
1	A	356	ASN
2	B	268	ASN
2	B	295	HIS
1	C	307	GLN
1	C	328	GLN
1	C	356	ASN
2	D	268	ASN
2	D	295	HIS
1	E	307	GLN
1	E	356	ASN
2	F	308	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

9 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	SO4	A	606	-	4,4,4	1.25	0	6,6,6	0.08	0
3	SO4	B	601	-	4,4,4	1.35	0	6,6,6	0.07	0
3	SO4	B	607	-	4,4,4	2.03	2 (50%)	6,6,6	0.07	0
3	SO4	C	605	-	4,4,4	1.21	0	6,6,6	0.09	0
3	SO4	D	603	-	4,4,4	1.29	0	6,6,6	0.08	0
3	SO4	D	608	-	4,4,4	2.24	4 (100%)	6,6,6	0.09	0
3	SO4	E	604	-	4,4,4	1.17	0	6,6,6	0.09	0
3	SO4	F	602	-	4,4,4	1.41	0	6,6,6	0.11	0
3	SO4	F	609	-	4,4,4	2.27	4 (100%)	6,6,6	0.07	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	SO4	A	606	-	-	0/0/0/0	0/0/0/0
3	SO4	B	601	-	-	0/0/0/0	0/0/0/0
3	SO4	B	607	-	-	0/0/0/0	0/0/0/0
3	SO4	C	605	-	-	0/0/0/0	0/0/0/0
3	SO4	D	603	-	-	0/0/0/0	0/0/0/0
3	SO4	D	608	-	-	0/0/0/0	0/0/0/0
3	SO4	E	604	-	-	0/0/0/0	0/0/0/0
3	SO4	F	602	-	-	0/0/0/0	0/0/0/0
3	SO4	F	609	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	607	SO4	O4-S	2.01	1.54	1.47
3	D	608	SO4	O4-S	2.01	1.54	1.47
3	F	609	SO4	O3-S	2.07	1.54	1.47
3	D	608	SO4	O3-S	2.10	1.54	1.47
3	F	609	SO4	O4-S	2.25	1.55	1.47
3	D	608	SO4	O1-S	2.25	1.54	1.47
3	F	609	SO4	O1-S	2.29	1.55	1.47
3	B	607	SO4	O2-S	2.36	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	609	SO4	O2-S	2.47	1.55	1.47
3	D	608	SO4	O2-S	2.57	1.55	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	607	SO4	1	0
3	C	605	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	101/101 (100%)	-0.09	1 (0%) 84 79	37, 63, 101, 117	0
1	C	101/101 (100%)	0.11	0 100 100	39, 67, 97, 114	0
1	E	101/101 (100%)	0.03	1 (0%) 84 79	46, 73, 104, 120	0
2	B	107/107 (100%)	0.26	3 (2%) 56 49	39, 69, 122, 140	0
2	D	106/107 (99%)	0.53	11 (10%) 8 5	43, 76, 129, 139	0
2	F	105/107 (98%)	0.40	11 (10%) 8 5	44, 74, 124, 139	0
All	All	621/624 (99%)	0.21	27 (4%) 39 31	37, 71, 119, 140	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	225	ALA	5.6
2	B	225	ALA	5.5
2	F	299	ILE	3.5
2	F	225	ALA	3.3
2	B	331	ASP	3.3
1	A	278	THR	3.2
2	D	299	ILE	3.2
2	B	267	GLU	3.1
2	F	303	VAL	3.1
2	F	301	ARG	3.1
2	D	267	GLU	3.0
2	D	226	SER	2.8
2	D	330	GLU	2.8
2	F	325	TYR	2.7
2	D	296	LYS	2.6
1	E	278	THR	2.4
2	D	303	VAL	2.4
2	D	265	ASP	2.4
2	F	300	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	329	VAL	2.3
2	F	329	VAL	2.2
2	D	300	GLU	2.2
2	F	323	PHE	2.2
2	D	275	ASP	2.2
2	F	297	MET	2.2
2	F	237	ALA	2.0
2	F	328	VAL	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	D	603	5/5	0.96	0.40	4.29	41,43,45,60	5
3	SO4	B	601	5/5	0.94	0.29	2.59	31,39,41,49	5
3	SO4	F	602	5/5	0.95	0.20	2.58	30,37,41,49	5
3	SO4	D	608	5/5	0.72	0.38	-	24,29,37,90	5
3	SO4	A	606	5/5	0.95	0.13	-	41,41,48,56	5
3	SO4	F	609	5/5	0.86	0.31	-	23,30,34,92	5
3	SO4	B	607	5/5	0.88	0.38	-	25,27,35,75	5
3	SO4	E	604	5/5	0.95	0.17	-	40,40,46,47	5
3	SO4	C	605	5/5	0.93	0.21	-	42,49,55,59	5

6.5 Other polymers (i)

There are no such residues in this entry.