Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 12:57 AM EDT

PDB ID	:	6ERH
Title	:	Complex of XLF and heterodimer Ku bound to DNA
Authors	:	Nemoz, C.; Legrand, P.; Ropars, V.; Charbonnier, J.B.
Deposited on	:	2017-10-18
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

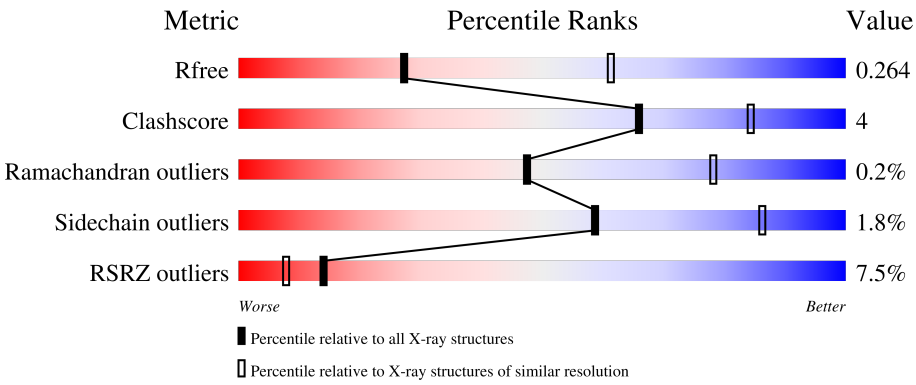
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	544	10% 79% 11% 10%
1	C	544	4% 81% 10% 9%
2	B	572	8% 81% 11% • 7%
2	D	572	6% 83% 9% • 6%
3	F	34	9% 76% 15% • 6%

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Mol	Chain	Length	Quality of chain
3	O	34	12% 71% 18% 12%
4	K	21	5% 52% 48%
4	R	21	5% 57% 43%
5	M	19	37% 63%
5	T	19	21% 11% 68%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 18810 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	490	3955	2531	672	735	17	0	0	0
1	C	493	3980	2547	677	738	18	0	0	0

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	534	4301	2746	734	797	24	0	0	0
2	D	535	4310	2752	736	798	24	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP P13010
B	-15	HIS	-	expression tag	UNP P13010
B	-14	HIS	-	expression tag	UNP P13010
B	-13	HIS	-	expression tag	UNP P13010
B	-12	HIS	-	expression tag	UNP P13010
B	-11	HIS	-	expression tag	UNP P13010
B	-10	HIS	-	expression tag	UNP P13010
B	-9	HIS	-	expression tag	UNP P13010
B	-8	HIS	-	expression tag	UNP P13010
B	-7	HIS	-	expression tag	UNP P13010
B	-6	HIS	-	expression tag	UNP P13010
B	-5	GLU	-	expression tag	UNP P13010
B	-4	ASN	-	expression tag	UNP P13010
B	-3	LEU	-	expression tag	UNP P13010
B	-2	TYR	-	expression tag	UNP P13010
B	-1	PHE	-	expression tag	UNP P13010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLN	-	expression tag	UNP P13010
B	1	GLY	-	expression tag	UNP P13010
D	-16	MET	-	initiating methionine	UNP P13010
D	-15	HIS	-	expression tag	UNP P13010
D	-14	HIS	-	expression tag	UNP P13010
D	-13	HIS	-	expression tag	UNP P13010
D	-12	HIS	-	expression tag	UNP P13010
D	-11	HIS	-	expression tag	UNP P13010
D	-10	HIS	-	expression tag	UNP P13010
D	-9	HIS	-	expression tag	UNP P13010
D	-8	HIS	-	expression tag	UNP P13010
D	-7	HIS	-	expression tag	UNP P13010
D	-6	HIS	-	expression tag	UNP P13010
D	-5	GLU	-	expression tag	UNP P13010
D	-4	ASN	-	expression tag	UNP P13010
D	-3	LEU	-	expression tag	UNP P13010
D	-2	TYR	-	expression tag	UNP P13010
D	-1	PHE	-	expression tag	UNP P13010
D	0	GLN	-	expression tag	UNP P13010
D	1	GLY	-	expression tag	UNP P13010

- Molecule 3 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	F	32	646	309	123	183	31	0	0	0
			Total	C	N	O	P			
3	O	30	610	290	118	172	30	0	0	0

- Molecule 4 is a DNA chain called DNA (21-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	K	21	431	208	71	132	20	0	0	0
			Total	C	N	O	P			
4	R	21	431	208	71	132	20	0	0	0

- Molecule 5 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	M	7	56	37	11	8	0	0	0

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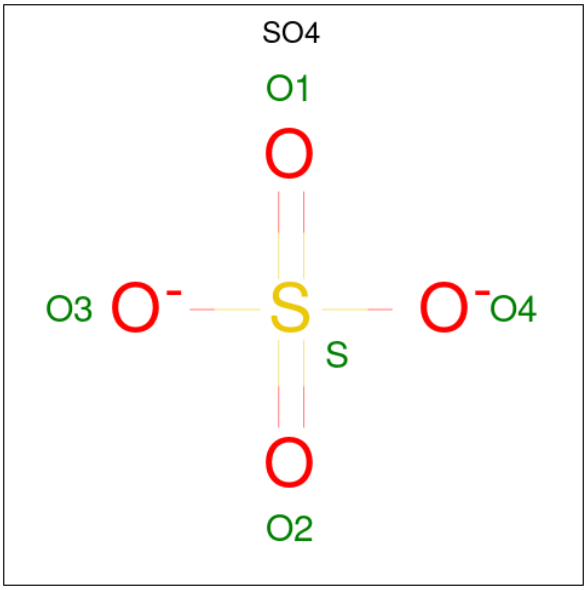
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	T	6	47	31	9	7	0	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	6	6	6	0	0
7	B	5	5	5	0	0
7	C	8	8	8	0	0
7	D	8	8	8	0	0
7	F	2	2	2	0	0
7	O	2	2	2	0	0

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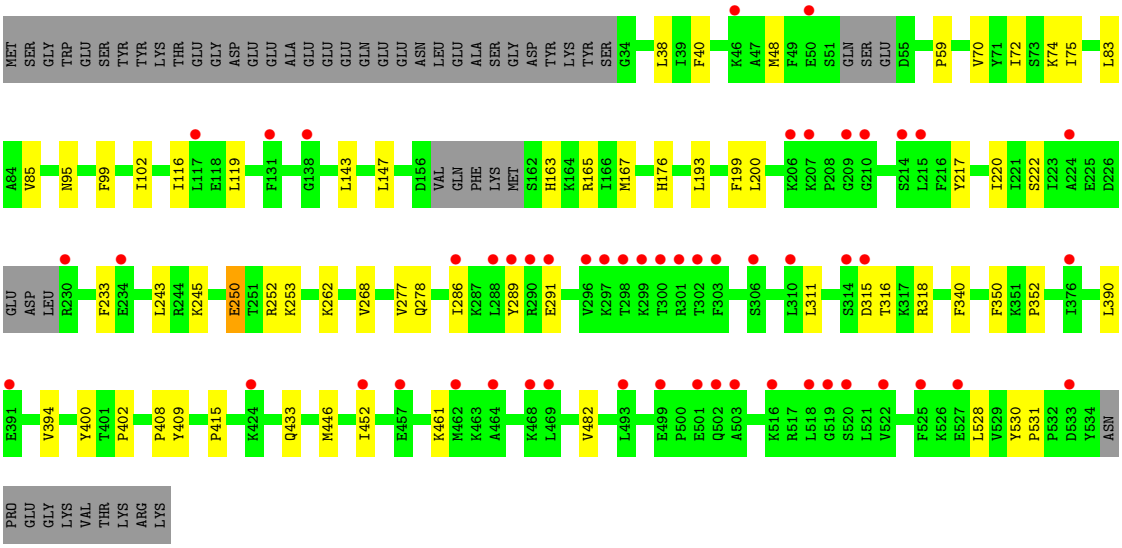
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	R	2	2	2	0	0

3 Residue-property plots (i)

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

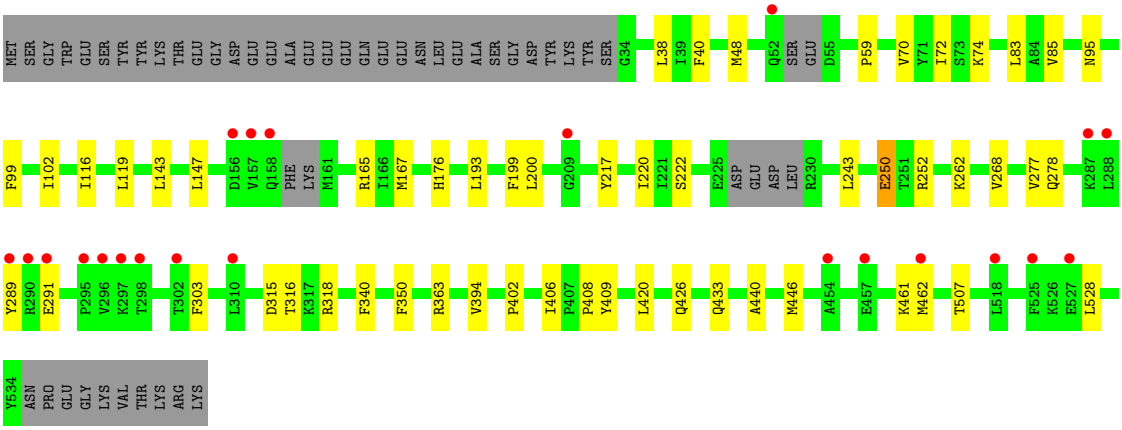
• Molecule 1: X-ray repair cross-complementing protein 6

Chain A:



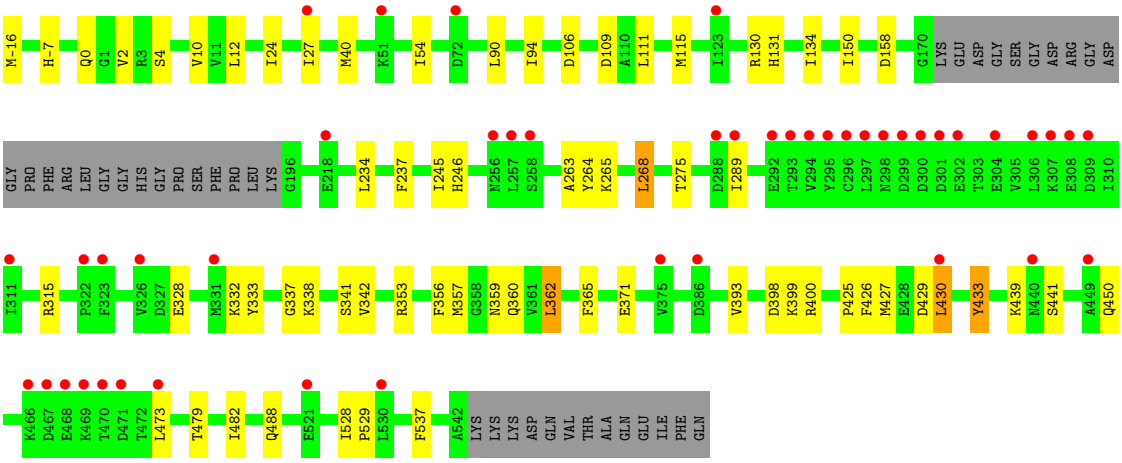
• Molecule 1: X-ray repair cross-complementing protein 6

Chain C:



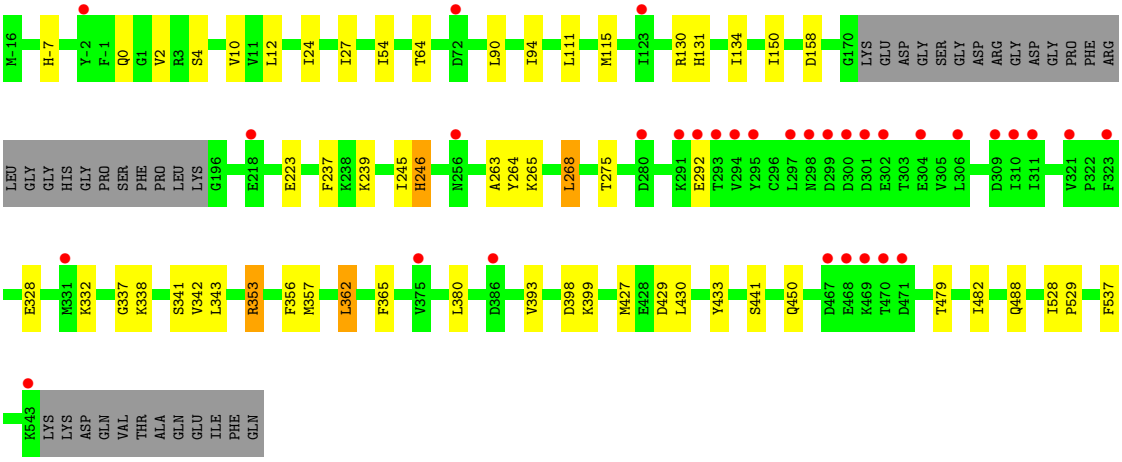
• Molecule 2: X-ray repair cross-complementing protein 5

Chain B:



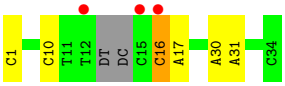
- Molecule 2: X-ray repair cross-complementing protein 5

Chain D:



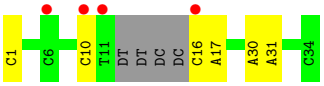
- Molecule 3: DNA (34-MER)

Chain F:



- Molecule 3: DNA (34-MER)

Chain O:

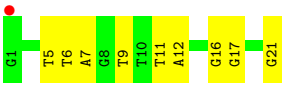


- Molecule 4: DNA (21-MER)

Chain K:

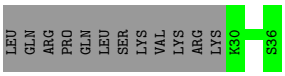
• Molecule 4: DNA (21-MER)

Chain R:



• Molecule 5: Non-homologous end-joining factor 1

Chain M:



• Molecule 5: Non-homologous end-joining factor 1

Chain T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.85Å 118.92Å 128.22Å 90.00° 93.11° 90.00°	Depositor
Resolution (Å)	49.38 – 2.80 49.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	50.4 (49.38-2.80) 50.4 (49.00-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.225 , 0.252 0.240 , 0.264	Depositor DCC
R_{free} test set	1918 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å^2)	62.9	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18810	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9723e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.34	0/4030	0.57	0/5426
1	C	0.35	0/4055	0.58	0/5459
2	B	0.33	0/4394	0.59	0/5929
2	D	0.34	0/4403	0.61	0/5940
3	F	1.02	1/724 (0.1%)	0.93	1/1110 (0.1%)
3	O	0.97	0/684	0.94	0/1048
4	K	0.97	0/481	1.00	0/743
4	R	0.94	0/481	1.01	0/743
5	M	0.49	0/57	0.77	0/74
5	T	0.37	0/48	0.77	0/62
All	All	0.47	1/19357 (0.0%)	0.65	1/26534 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	16	DC	C3'-O3'	5.96	1.51	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	16	DC	P-O3'-C3'	5.19	125.93	119.70

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	3955	0	4034	38	0
1	C	3980	0	4064	33	0
2	B	4301	0	4308	43	0
2	D	4310	0	4321	37	0
3	F	646	0	360	5	0
3	O	610	0	336	4	0
4	K	431	0	243	9	0
4	R	431	0	243	6	0
5	M	56	0	60	0	0
5	T	47	0	48	2	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
7	A	6	0	0	0	0
7	B	5	0	0	0	0
7	C	8	0	0	0	0
7	D	8	0	0	0	0
7	F	2	0	0	0	0
7	O	2	0	0	0	0
7	R	2	0	0	0	0
All	All	18810	0	18017	146	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 4.

All (146) 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)
2:D:263:ALA:HB1	2:D:362:LEU:HD22	1.41	0.97
2:B:263:ALA:HB1	2:B:362:LEU:HD22	1.50	0.92
1:C:446:MET:HE1	2:D:264:TYR:HB2	1.62	0.82
2:D:263:ALA:HB1	2:D:362:LEU:CD2	2.15	0.77
2:B:400:ARG:HH12	4:K:13:DT:H4'	1.51	0.75
1:A:143:LEU:H	1:A:176:HIS:HE1	1.37	0.73
1:C:143:LEU:H	1:C:176:HIS:HE1	1.36	0.72
3:O:1:DC:H5	4:R:21:DG:H22	1.40	0.68
1:A:350:PHE:HB3	1:A:394:VAL:CG1	2.26	0.65
1:A:350:PHE:HB3	1:A:394:VAL:HG11	1.78	0.65
2:D:24:ILE:HD12	2:D:27:ILE:HD11	1.79	0.64
1:C:350:PHE:HB3	1:C:394:VAL:CG1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:LYS:HG2	2:B:398:ASP:HA	1.80	0.64
2:D:338:LYS:HG2	2:D:398:ASP:HA	1.79	0.64
2:B:263:ALA:HB1	2:B:362:LEU:CD2	2.25	0.64
1:C:350:PHE:HB3	1:C:394:VAL:HG11	1.79	0.64
2:B:24:ILE:HD12	2:B:27:ILE:HD11	1.80	0.63
2:B:111:LEU:HD13	2:B:134:ILE:HD11	1.81	0.63
1:C:40:PHE:HE2	1:C:83:LEU:HD23	1.65	0.62
1:A:40:PHE:HE2	1:A:83:LEU:HD23	1.63	0.61
2:B:328:GLU:O	2:B:332:LYS:HB2	2.00	0.61
2:B:0:GLN:HA	2:B:4:SER:HB3	1.81	0.61
2:D:265:LYS:HD3	2:D:268:LEU:HD11	1.82	0.61
2:B:265:LYS:HD3	2:B:268:LEU:HD11	1.81	0.61
2:D:111:LEU:HD13	2:D:134:ILE:HD11	1.81	0.60
1:C:446:MET:CE	2:D:264:TYR:HB2	2.30	0.60
3:F:10:DC:H42	3:F:17:DA:H61	1.50	0.60
2:D:328:GLU:O	2:D:332:LYS:HB2	2.02	0.60
3:F:1:DC:H5	4:K:21:DG:H22	1.49	0.59
2:D:0:GLN:HA	2:D:4:SER:HB3	1.82	0.59
1:A:446:MET:HE1	2:B:264:TYR:HB2	1.84	0.59
1:A:446:MET:HE2	2:B:365:PHE:HE2	1.67	0.58
1:A:253:LYS:HG2	2:B:433:TYR:HB3	1.85	0.58
1:C:316:THR:HG23	1:C:318:ARG:HH12	1.69	0.58
2:B:400:ARG:NH1	4:K:13:DT:H4'	2.17	0.57
1:C:48:MET:HA	1:C:59:PRO:HG2	1.86	0.57
2:D:237:PHE:H	2:D:488:GLN:HE22	1.52	0.57
3:O:10:DC:H42	3:O:17:DA:H61	1.52	0.57
1:A:48:MET:HA	1:A:59:PRO:HG2	1.86	0.57
1:A:278:GLN:HE22	4:K:5:DT:H3'	1.69	0.56
2:B:90:LEU:O	2:B:94:ILE:HG12	2.04	0.56
2:D:342:VAL:HA	2:D:393:VAL:HG12	1.87	0.56
2:D:90:LEU:O	2:D:94:ILE:HG12	2.06	0.56
2:B:2:VAL:HG21	2:B:245:ILE:HD13	1.88	0.56
2:B:237:PHE:H	2:B:488:GLN:HE22	1.52	0.56
2:B:342:VAL:HA	2:B:393:VAL:HG12	1.87	0.56
2:B:479:THR:HA	2:B:482:ILE:HD12	1.88	0.55
2:D:2:VAL:HG21	2:D:245:ILE:HD13	1.88	0.55
1:A:316:THR:HG23	1:A:318:ARG:HH12	1.71	0.55
1:C:433:GLN:HE22	2:D:353:ARG:HG3	1.70	0.55
2:D:479:THR:HA	2:D:482:ILE:HD12	1.88	0.54
2:B:337:GLY:HA2	2:B:399:LYS:HA	1.89	0.54
2:D:427:MET:O	2:D:430:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:PRO:HG3	2:B:473:LEU:HD21	1.90	0.53
1:C:446:MET:HE2	2:D:365:PHE:HE2	1.73	0.52
2:D:337:GLY:HA2	2:D:399:LYS:HA	1.91	0.52
2:B:275:THR:HG21	4:K:9:DT:H5'	1.92	0.51
2:B:426:PHE:O	2:B:429:ASP:OD1	2.27	0.51
2:D:265:LYS:HB3	2:D:268:LEU:HD11	1.93	0.51
1:A:340:PHE:HB2	1:A:408:PRO:HD3	1.92	0.50
3:F:16:DC:H4'	3:F:17:DA:OP1	2.12	0.50
1:C:340:PHE:HB2	1:C:408:PRO:HD3	1.92	0.50
2:B:528:ILE:HB	2:B:529:PRO:HD3	1.94	0.50
2:B:265:LYS:HB3	2:B:268:LEU:HD11	1.93	0.50
2:D:-7:HIS:O	2:D:2:VAL:HG22	2.12	0.49
2:B:-7:HIS:O	2:B:2:VAL:HG22	2.12	0.49
2:B:425:PRO:HB2	2:B:429:ASP:OD1	2.12	0.49
1:A:433:GLN:HE22	2:B:353:ARG:HG3	1.77	0.49
1:C:217:TYR:HA	1:C:220:ILE:HB	1.94	0.49
2:B:353:ARG:HA	2:B:356:PHE:CD1	2.48	0.48
1:A:446:MET:CE	2:B:365:PHE:HE2	2.27	0.48
1:A:446:MET:CE	2:B:264:TYR:HB2	2.44	0.48
2:B:400:ARG:HH12	4:K:13:DT:C4'	2.24	0.48
2:D:528:ILE:HB	2:D:529:PRO:HD3	1.95	0.48
1:C:278:GLN:HE22	4:R:5:DT:H3'	1.79	0.47
1:A:452:ILE:HD13	2:B:371:GLU:HG3	1.95	0.47
1:C:147:LEU:HB3	1:C:193:LEU:HD11	1.96	0.47
2:D:353:ARG:HA	2:D:356:PHE:CD1	2.49	0.47
1:A:482:VAL:HG22	2:B:333:TYR:HD2	1.80	0.47
1:A:217:TYR:HA	1:A:220:ILE:HB	1.97	0.47
1:C:143:LEU:H	1:C:176:HIS:CE1	2.26	0.46
1:C:193:LEU:HD13	1:C:200:LEU:HD21	1.96	0.46
1:A:147:LEU:HB3	1:A:193:LEU:HD11	1.96	0.46
1:C:95:ASN:ND2	1:C:102:ILE:HB	2.30	0.46
1:A:165:ARG:HG3	1:A:199:PHE:HB2	1.98	0.46
4:R:6:DT:H2"	4:R:7:DA:C8	2.50	0.46
1:A:193:LEU:HD13	1:A:200:LEU:HD21	1.98	0.46
1:A:311:LEU:HD13	2:B:289:ILE:HD12	1.98	0.46
1:C:38:LEU:HD22	1:C:250:GLU:HG2	1.97	0.46
1:C:165:ARG:HG3	1:C:199:PHE:HB2	1.98	0.46
4:K:6:DT:H2"	4:K:7:DA:C8	2.50	0.46
1:A:163:HIS:HB2	1:A:252:ARG:NH1	2.30	0.46
1:A:38:LEU:HD22	1:A:250:GLU:HG2	1.97	0.46
1:C:462:MET:HG2	2:D:380:LEU:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LYS:HG3	1:A:528:LEU:HD12	1.98	0.45
1:C:303:PHE:HE2	2:D:292:GLU:HB2	1.80	0.45
2:D:275:THR:HG21	4:R:9:DT:H5'	1.98	0.45
1:C:440:ALA:O	2:D:239:LYS:HE3	2.16	0.45
1:A:72:ILE:HG12	1:A:116:ILE:HD13	1.98	0.45
1:A:95:ASN:ND2	1:A:102:ILE:HB	2.31	0.45
1:C:507:THR:O	2:D:343:LEU:HD21	2.16	0.45
1:C:461:LYS:HG3	1:C:528:LEU:HD12	1.99	0.44
2:D:10:VAL:HG22	2:D:131:HIS:HB2	1.99	0.44
2:B:115:MET:HE2	2:B:150:ILE:HG23	2.00	0.44
2:B:10:VAL:HG22	2:B:131:HIS:HB2	1.99	0.44
4:R:11:DT:H2"	4:R:12:DA:C8	2.53	0.44
2:B:450:GLN:HB3	2:B:537:PHE:CZ	2.53	0.44
1:A:286:ILE:HD13	2:B:315:ARG:HG3	2.00	0.43
2:D:115:MET:HE2	2:D:150:ILE:HG23	1.99	0.43
1:C:95:ASN:ND2	1:C:99:PHE:HB2	2.32	0.43
4:R:16:DG:H2"	4:R:17:DG:C8	2.53	0.43
4:K:11:DT:H2"	4:K:12:DA:C8	2.53	0.43
1:A:262:LYS:HG2	1:A:268:VAL:HG22	2.01	0.43
4:K:16:DG:H2"	4:K:17:DG:C8	2.54	0.43
1:A:95:ASN:ND2	1:A:99:PHE:HB2	2.32	0.43
2:B:427:MET:O	2:B:430:LEU:HG	2.19	0.43
1:A:85:VAL:HG21	1:A:119:LEU:HD21	2.00	0.43
1:C:72:ILE:HG12	1:C:116:ILE:HD13	2.01	0.43
1:C:262:LYS:HG2	1:C:268:VAL:HG22	2.01	0.43
3:F:16:DC:H2"	3:F:17:DA:C5	2.54	0.43
1:C:85:VAL:HG21	1:C:119:LEU:HD21	2.00	0.42
2:B:130:ARG:HH21	2:B:158:ASP:HB3	1.83	0.42
2:D:130:ARG:HH21	2:D:158:ASP:HB3	1.85	0.42
1:C:446:MET:CE	2:D:365:PHE:HE2	2.32	0.42
2:D:131:HIS:CD2	5:T:33:GLY:HA2	2.55	0.42
3:O:16:DC:H5"	3:O:17:DA:OP1	2.19	0.42
2:D:450:GLN:HB3	2:D:537:PHE:CZ	2.54	0.42
1:A:70:VAL:O	1:A:74:LYS:HG2	2.20	0.42
1:A:400:TYR:CE2	1:A:402:PRO:HG3	2.55	0.42
2:B:40:MET:HB3	2:B:234:LEU:HB3	2.02	0.42
2:B:12:LEU:HD11	2:B:54:ILE:HD11	2.02	0.41
2:B:106:ASP:HB3	2:B:109:ASP:HB2	2.02	0.41
1:A:530:TYR:HA	1:A:531:PRO:HD3	1.96	0.41
3:F:30:DA:H2"	3:F:31:DA:C8	2.56	0.41
1:A:289:TYR:CE2	1:A:291:GLU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LEU:HG	1:A:415:PRO:HB2	2.03	0.41
1:C:70:VAL:O	1:C:74:LYS:HG2	2.20	0.41
2:D:12:LEU:HD11	2:D:54:ILE:HD11	2.03	0.41
1:A:75:ILE:HD12	1:A:116:ILE:HD11	2.03	0.40
1:C:289:TYR:CE2	1:C:291:GLU:HB2	2.57	0.40
1:C:402:PRO:HD2	1:C:406:ILE:HG21	2.04	0.40
1:A:233:PHE:CD2	1:A:245:LYS:HG2	2.56	0.40
1:C:420:LEU:HD23	1:C:426:GLN:HA	2.03	0.40
3:O:30:DA:H2"	3:O:31:DA:C8	2.56	0.40
2:D:223:GLU:HG3	5:T:32:ARG:HH21	1.86	0.40
2:D:246:HIS:HB2	2:D:264:TYR:CE1	2.56	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	482/544 (89%)	467 (97%)	14 (3%)	1 (0%)	47	78
1	C	485/544 (89%)	470 (97%)	14 (3%)	1 (0%)	47	78
2	B	530/572 (93%)	512 (97%)	17 (3%)	1 (0%)	47	78
2	D	531/572 (93%)	512 (96%)	17 (3%)	2 (0%)	34	66
5	M	5/19 (26%)	5 (100%)	0	0	100	100
5	T	4/19 (21%)	4 (100%)	0	0	100	100
All	All	2037/2270 (90%)	1970 (97%)	62 (3%)	5 (0%)	47	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	441	SER

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Mol	Chain	Res	Type
2	B	433	TYR
2	D	433	TYR
1	C	250	GLU
1	A	250	GLU

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	444/492 (90%)	438 (99%)	6 (1%)	67	90
1	C	447/492 (91%)	439 (98%)	8 (2%)	59	86
2	B	483/513 (94%)	472 (98%)	11 (2%)	50	82
2	D	484/513 (94%)	476 (98%)	8 (2%)	60	87
5	M	6/18 (33%)	6 (100%)	0	100	100
5	T	5/18 (28%)	5 (100%)	0	100	100
All	All	1869/2046 (91%)	1836 (98%)	33 (2%)	59	86

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

Mol	Chain	Res	Type
1	A	167	MET
1	A	222	SER
1	A	243	LEU
1	A	277	VAL
1	A	315	ASP
1	A	409	TYR
2	B	-16	MET
2	B	246	HIS
2	B	268	LEU
2	B	341	SER
2	B	357	MET
2	B	359	ASN
2	B	360	GLN
2	B	362	LEU

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Mol	Chain	Res	Type
2	B	430	LEU
2	B	439	LYS
2	B	441	SER
1	C	167	MET
1	C	222	SER
1	C	243	LEU
1	C	252	ARG
1	C	277	VAL
1	C	315	ASP
1	C	363	ARG
1	C	409	TYR
2	D	64	THR
2	D	246	HIS
2	D	268	LEU
2	D	341	SER
2	D	353	ARG
2	D	357	MET
2	D	362	LEU
2	D	429	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	HIS
1	A	433	GLN
2	B	-12	HIS
2	B	-9	HIS
2	B	-8	HIS
2	B	73	GLN
2	B	131	HIS
2	B	488	GLN
1	C	176	HIS
1	C	433	GLN
2	D	-12	HIS
2	D	-9	HIS
2	D	-8	HIS
2	D	73	GLN
2	D	131	HIS
2	D	488	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
6	SO4	A	601	-	4,4,4	0.25	0	6,6,6	0.09	0
6	SO4	C	601	-	4,4,4	0.25	0	6,6,6	0.19	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.

No monomer is involved in short contacts.

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(Å^2)	Q<0.9
1	A	490/544 (90%)	0.63	53 (10%)	5	3	36, 92, 166, 194	0
1	C	493/544 (90%)	0.31	22 (4%)	33	23	26, 72, 153, 178	0
2	B	534/572 (93%)	0.50	45 (8%)	11	5	30, 78, 151, 190	0
2	D	535/572 (93%)	0.38	33 (6%)	20	13	25, 73, 130, 187	0
3	F	32/34 (94%)	0.78	3 (9%)	8	4	52, 126, 175, 190	0
3	O	30/34 (88%)	0.80	4 (13%)	3	2	50, 108, 160, 181	0
4	K	21/21 (100%)	-0.02	1 (4%)	30	21	71, 90, 147, 164	0
4	R	21/21 (100%)	0.32	1 (4%)	30	21	65, 91, 140, 155	0
5	M	7/19 (36%)	0.10	0	100	100	41, 45, 75, 83	0
5	T	6/19 (31%)	-0.10	0	100	100	39, 44, 67, 73	0
All	All	2169/2380 (91%)	0.46	162 (7%)	14	8	25, 80, 155, 194	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	157	VAL	8.2
2	B	470	THR	6.9
2	D	470	THR	6.9
2	D	301	ASP	6.5
1	A	527	GLU	6.5
1	A	289	TYR	6.4
2	B	298	ASN	6.3
1	A	291	GLU	6.2
2	B	440	ASN	6.1
3	F	15	DC	5.9
1	C	290	ARG	5.9
2	B	294	VAL	5.9
3	F	12	DT	5.4

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Mol	Chain	Res	Type	RSRZ
2	B	467	ASP	5.3
1	C	288	LEU	5.2
1	A	298	THR	5.2
2	B	296	CYS	5.2
2	B	292	GLU	5.1
2	B	331	MET	5.1
2	B	469	LYS	5.0
2	D	302	GLU	4.8
1	C	158	GLN	4.8
1	A	209	GLY	4.8
1	C	289	TYR	4.8
2	B	304	GLU	4.6
2	B	297	LEU	4.6
1	A	457	GLU	4.6
2	D	467	ASP	4.6
1	A	306	SER	4.6
1	A	288	LEU	4.5
1	A	299	LYS	4.5
2	B	295	TYR	4.4
2	B	256	ASN	4.3
1	A	493	LEU	4.2
1	A	234	GLU	4.2
2	B	288	ASP	4.2
2	D	469	LYS	4.1
2	B	468	GLU	4.1
1	A	290	ARG	4.1
1	A	501	GLU	4.1
1	A	224	ALA	4.0
1	C	454	ALA	4.0
2	D	256	ASN	4.0
1	C	209	GLY	3.9
1	A	297	LYS	3.9
1	C	310	LEU	3.8
1	C	296	VAL	3.8
2	B	72	ASP	3.8
1	A	468	LYS	3.7
2	D	299	ASP	3.7
2	D	310	ILE	3.6
2	B	473	LEU	3.6
2	B	289	ILE	3.6
2	D	468	GLU	3.6
4	R	1	DG	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	72	ASP	3.5
1	A	499	GLU	3.5
2	B	323	PHE	3.5
2	D	386	ASP	3.5
2	D	123	ILE	3.4
2	B	293	THR	3.4
1	C	302	THR	3.4
3	F	16	DC	3.4
1	C	457	GLU	3.4
1	A	214	SER	3.3
2	B	299	ASP	3.3
1	A	303	PHE	3.3
2	B	301	ASP	3.3
1	C	52	GLN	3.3
2	B	471	ASP	3.3
2	B	27	ILE	3.3
1	C	295	PRO	3.2
1	A	314	SER	3.2
2	D	280	ASP	3.1
2	B	309	ASP	3.1
1	C	297	LYS	3.1
1	A	522	VAL	3.0
2	B	375	VAL	3.0
2	D	292	GLU	3.0
1	A	215	LEU	2.9
2	D	311	ILE	2.9
1	A	210	GLY	2.9
1	A	464	ALA	2.9
1	A	469	LEU	2.9
2	B	521	GLU	2.9
1	A	50	GLU	2.9
1	A	452	ILE	2.9
3	O	16	DC	2.8
1	A	296	VAL	2.8
1	A	301	ARG	2.8
1	A	230	ARG	2.8
1	A	519	GLY	2.8
2	D	543	LYS	2.8
1	C	462	MET	2.8
2	D	295	TYR	2.8
2	B	123	ILE	2.8
2	B	308	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	291	GLU	2.7
1	A	46	LYS	2.7
2	B	307	LYS	2.6
1	A	520	SER	2.6
1	A	300	THR	2.6
1	A	302	THR	2.6
3	O	10	DC	2.6
2	D	297	LEU	2.5
2	D	309	ASP	2.5
2	B	300	ASP	2.5
2	D	291	LYS	2.5
1	A	516	LYS	2.5
1	C	287	LYS	2.5
1	C	527	GLU	2.5
1	C	518	LEU	2.5
2	D	304	GLU	2.5
2	D	331	MET	2.5
1	A	315	ASP	2.5
1	C	298	THR	2.5
2	D	321	VAL	2.5
1	A	502	GLN	2.5
2	B	322	PRO	2.4
2	D	323	PHE	2.4
2	B	530	LEU	2.4
1	A	533	ASP	2.4
1	A	503	ALA	2.4
1	A	206	LYS	2.4
1	A	310	LEU	2.4
1	A	424	LYS	2.4
2	D	471	ASP	2.3
2	D	300	ASP	2.3
1	C	525	PHE	2.3
1	A	117	LEU	2.3
1	A	138	GLY	2.3
2	B	311	ILE	2.3
1	A	462	MET	2.2
1	A	391	GLU	2.2
2	D	293	THR	2.2
1	A	518	LEU	2.2
1	A	286	ILE	2.2
2	B	326	VAL	2.2
2	B	466	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	257	LEU	2.2
2	B	386	ASP	2.2
2	B	258	SER	2.2
1	A	376	ILE	2.2
2	B	218	GLU	2.2
2	D	298	ASN	2.2
2	D	375	VAL	2.2
2	D	218	GLU	2.1
3	O	6	DC	2.1
2	B	51	LYS	2.1
2	D	294	VAL	2.1
1	A	131	PHE	2.1
1	A	525	PHE	2.1
2	B	430	LEU	2.1
2	B	449	ALA	2.1
3	O	11	DT	2.1
1	C	156	ASP	2.0
4	K	1	DG	2.0
2	B	302	GLU	2.0
2	D	-2	TYR	2.0
2	B	306	LEU	2.0
1	A	207	LYS	2.0
2	D	306	LEU	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 monosaccharides 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. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	A	601	5/5	0.95	0.13	96,96,96,97	0
6	SO4	C	601	5/5	0.95	0.13	94,94,95,95	0

6.5 Other polymers (i)

There are no such residues in this entry.