Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 07:42 AM EDT

PDB ID	:	3MV8
Title	:	Crystal Structure of the TK3-Gln55His TCR in complex with HLA-B*3501/HPVG
Authors	:	Gras, S.; Chen, Z.; Miles, J.J.; Liu, Y.C.; Bell, M.J.; Sullivan, L.C.; Kjer-Nielsen, L.; Brennan, R.M.; Burrows, J.M.; Neller, M.A.; Khanna, R.; Purcell, A.W.; Brooks, A.G.; McCluskey, J.; Rossjohn, J.; Burrows, S.R.
Deposited on	:	2010-05-03
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

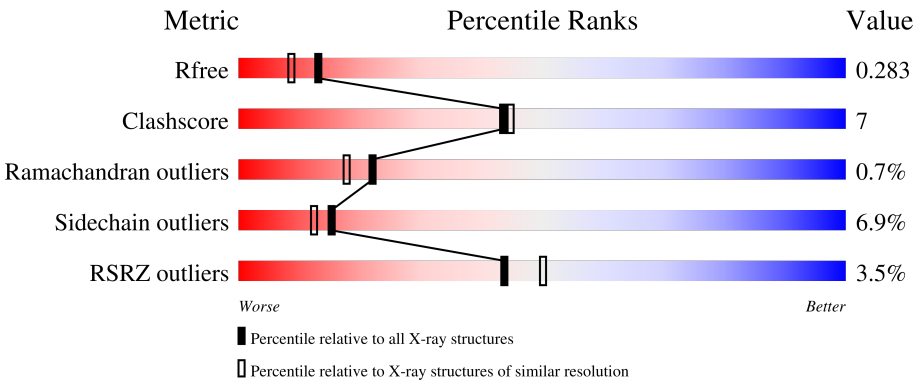
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	276	3% 85% 13% •
2	B	100	7% 76% 21% •
3	C	11	55% 45%
4	D	200	4% 76% 20% • •

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Mol	Chain	Length	Quality of chain
5	E	242	2% 83% 14%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7064 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 HLA class I histocompatibility antigen, B-35 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2320	1442	428	442	8	0	7	0

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	852	544	143	161	4	0	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	INITIATING METHIONINE	UNP P61769

- Molecule 3 is a protein called HPVG peptide from Epstein-Barr nuclear antigen 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	11	95	62	13	20	0	0	0

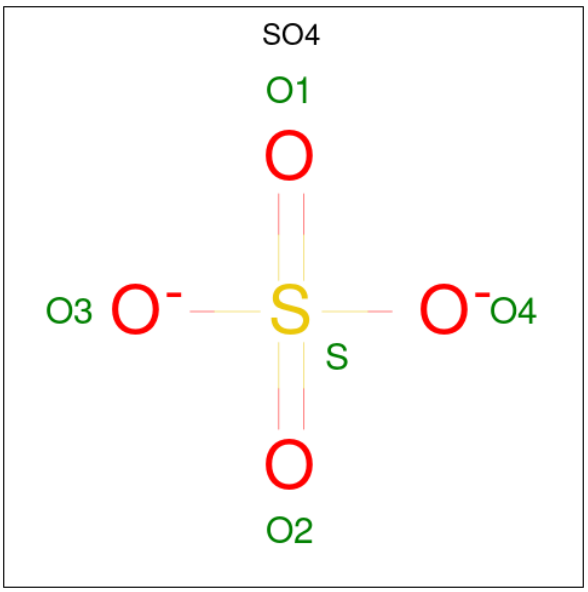
- Molecule 4 is a protein called alpha chain of the TK3 TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	200	1648	1024	274	343	7	0	11	0

- Molecule 5 is a protein called beta chain of the TK3 TCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	242	1943	1221	338	378	6	0	2	0

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



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

- Molecule 7 is water.

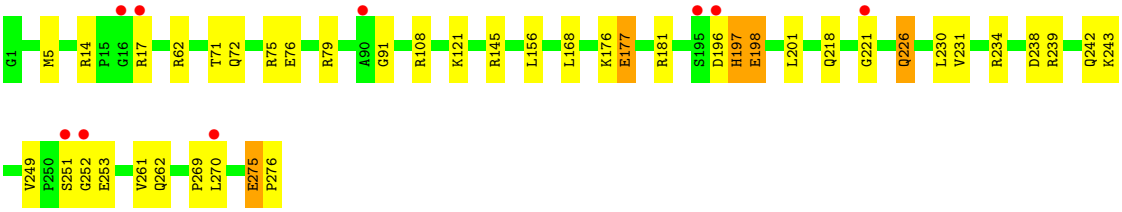
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	69	69	69	0	0
			Total	O		
7	B	14	14	14	0	0
			Total	O		
7	C	5	5	5	0	0
			Total	O		
7	D	66	66	66	0	0
			Total	O		
7	E	47	47	47	0	0

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.

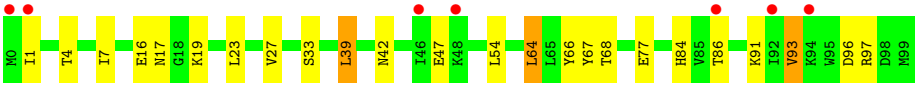
• Molecule 1: HLA class I histocompatibility antigen, B-35 alpha chain

Chain A:



• Molecule 2: Beta-2-microglobulin

Chain B:

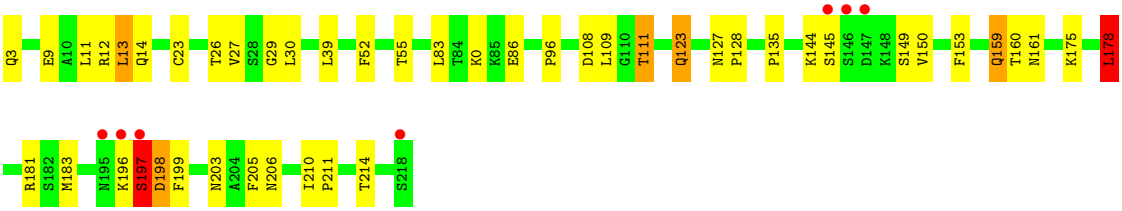


• Molecule 3: HPVG peptide from Epstein-Barr nuclear antigen 1

Chain C:

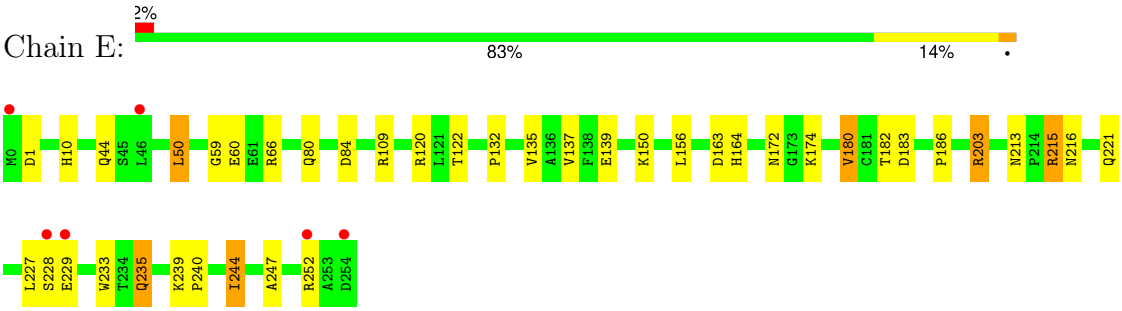
• Molecule 4: alpha chain of the TK3 TCR

Chain D:



• Molecule 5: beta chain of the TK3 TCR

Chain E:


2%
83%
14%
M0 D1 H10 Q44 S45 L46 L50 G59 E60 E61 R66 Q80 D84 R109 R120 L121 T122 P132 V135 A136 V137 F138 E139 K150 L156 D163 H164 N172 G173 K174 V180 C181 T182 D183 P186 R203 N213 P214 R215 N216 Q221
L227 S228 E229 W233 T234 Q235 K239 P240 T244 A247 R252 A253 D254

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	44.76Å 63.61Å 88.14Å 101.12° 97.60° 112.00°	Depositor
Resolution (Å)	84.22 – 2.10 84.27 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.2 (84.22-2.10) 98.2 (84.27-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.229 , 0.276 0.243 , 0.283	Depositor DCC
R_{free} test set	2513 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 29.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7064	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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, 0.333 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	0.35	0/2383	0.53	0/3237
2	B	0.36	0/875	0.53	0/1183
3	C	0.50	0/99	0.47	0/133
4	D	0.37	0/1680	0.60	1/2272 (0.0%)
5	E	0.36	0/1993	0.52	0/2708
All	All	0.36	0/7030	0.54	1/9533 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	178	LEU	CA-CB-CG	5.17	127.18	115.30

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	2320	0	2180	27	0
2	B	852	0	821	12	0
3	C	95	0	76	5	0
4	D	1648	0	1567	26	0
5	E	1943	0	1839	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	5	0	0	0	0
7	A	69	0	0	1	0
7	B	14	0	0	0	0
7	C	5	0	0	0	0
7	D	66	0	0	3	0
7	E	47	0	0	0	0
All	All	7064	0	6483	90	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 (90) 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:72[B]:GLN:HE21	5:E:60:GLU:CD	1.60	1.05
1:A:72[B]:GLN:NE2	5:E:60:GLU:CD	2.22	0.92
1:A:62:ARG:HE	3:C:1:HIS:HE1	1.18	0.87
5:E:10:HIS:ND1	5:E:164:HIS:HD2	1.79	0.80
4:D:14:GLN:NE2	4:D:127:ASN:HD22	1.81	0.77
4:D:108:ASP:HB3	4:D:111:THR:HG23	1.69	0.74
4:D:12[A]:ARG:HH22	4:D:123:GLN:HE22	1.35	0.74
2:B:4:THR:HA	2:B:86:THR:HG21	1.71	0.72
4:D:14:GLN:HE22	4:D:127:ASN:HD22	1.35	0.72
4:D:144:LYS:HB3	4:D:145:SER:HA	1.72	0.72
4:D:135:PRO:HB2	4:D:214[A]:THR:HG22	1.74	0.70
4:D:52:PHE:HZ	4:D:55[B]:THR:HG23	1.57	0.69
1:A:62:ARG:HE	3:C:1:HIS:CE1	2.07	0.69
4:D:12[B]:ARG:HH22	4:D:123:GLN:HE22	1.39	0.68
4:D:52:PHE:CZ	4:D:55[B]:THR:HG23	2.28	0.67
1:A:176:LYS:O	1:A:177:GLU:HB3	1.94	0.66
4:D:161:ASN:HB3	7:D:227:HOH:O	1.95	0.66
2:B:7:ILE:HG21	2:B:93[A]:VAL:HG21	1.79	0.65
5:E:122:THR:OG1	5:E:164:HIS:HE1	1.80	0.65
5:E:227:LEU:HD22	5:E:240:PRO:HD2	1.80	0.64
5:E:59:GLY:H	5:E:80:GLN:NE2	1.98	0.61
5:E:10:HIS:ND1	5:E:164:HIS:CD2	2.67	0.60
1:A:239:ARG:HH11	1:A:239:ARG:HA	1.66	0.59
2:B:7:ILE:CG2	2:B:93[A]:VAL:HG21	2.33	0.59
4:D:160:THR:HG21	4:D:211:PRO:HG3	1.85	0.57
4:D:203:ASN:O	4:D:206:ASN:HB2	2.05	0.56
2:B:33:SER:HB2	2:B:54:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:163:ASP:OD1	5:E:186:PRO:HG2	2.07	0.55
5:E:183:ASP:OD2	5:E:203:ARG:NH1	2.35	0.55
4:D:14:GLN:HE22	4:D:127:ASN:ND2	2.05	0.54
1:A:230:LEU:HD12	1:A:243:LYS:HE3	1.91	0.52
2:B:42:ASN:ND2	2:B:77:GLU:H	2.07	0.52
4:D:27[A]:VAL:HG13	4:D:108:ASP:CG	2.30	0.52
1:A:91:GLY:HA2	7:A:288:HOH:O	2.10	0.51
1:A:198:GLU:HG2	1:A:251:SER:HB3	1.91	0.51
3:C:1:HIS:HD2	3:C:2:PRO:O	1.94	0.51
1:A:72[B]:GLN:NE2	5:E:60:GLU:CG	2.74	0.50
2:B:27:VAL:HG22	2:B:64:LEU:HD12	1.93	0.50
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.93	0.50
4:D:12[A]:ARG:NH2	4:D:123:GLN:HE22	2.08	0.50
4:D:27[A]:VAL:HG12	4:D:29:GLY:N	2.27	0.50
2:B:84:HIS:ND1	2:B:86:THR:HG22	2.27	0.50
2:B:39:LEU:HD23	2:B:68:THR:HG22	1.93	0.49
4:D:197:SER:O	4:D:199:PHE:N	2.45	0.49
4:D:96:PRO:HG3	4:D:128:PRO:HB3	1.94	0.48
1:A:238:ASP:O	1:A:239:ARG:HB2	2.13	0.48
1:A:262:GLN:HE21	1:A:269:PRO:HG3	1.78	0.48
3:C:8:TYR:CD2	5:E:109:ARG:HA	2.49	0.47
5:E:44:GLN:HB2	5:E:50:LEU:CD1	2.45	0.47
4:D:23:CYS:O	4:D:86[A]:GLU:HB2	2.15	0.47
5:E:44:GLN:HB2	5:E:50:LEU:HD12	1.97	0.47
5:E:172:ASN:HD21	5:E:216:ASN:HD22	1.63	0.47
1:A:181:ARG:O	1:A:181:ARG:HG3	2.15	0.46
4:D:11:LEU:HD22	4:D:13:LEU:HD13	1.96	0.46
2:B:16:GLU:HB3	2:B:19:LYS:HB3	1.98	0.46
5:E:213:ASN:HD21	5:E:215:ARG:NH1	2.13	0.46
1:A:251:SER:O	1:A:253:GLU:N	2.48	0.46
4:D:144:LYS:N	4:D:145:SER:HB2	2.31	0.46
2:B:23:LEU:O	2:B:67:TYR:HA	2.16	0.46
2:B:17:ASN:ND2	2:B:97:ARG:HH12	2.15	0.45
2:B:64:LEU:HD13	2:B:66:TYR:CE2	2.51	0.45
4:D:210:ILE:HB	7:D:258:HOH:O	2.15	0.45
5:E:137:VAL:HG23	5:E:247:ALA:HB3	2.00	0.43
5:E:221:GLN:HG3	5:E:244:ILE:HD13	2.00	0.43
1:A:239:ARG:HA	1:A:239:ARG:NH1	2.33	0.43
1:A:198:GLU:CG	1:A:251:SER:HB3	2.48	0.43
1:A:76:GLU:HG3	1:A:79:ARG:NH2	2.34	0.43
1:A:201:LEU:HD12	1:A:249:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3:GLN:HG3	4:D:26:THR:O	2.19	0.42
5:E:120:ARG:HH22	5:E:163:ASP:HB3	1.84	0.42
5:E:132:PRO:HD3	5:E:240:PRO:HB3	2.02	0.42
5:E:233:TRP:CE2	5:E:235:GLN:HB2	2.54	0.42
1:A:261:VAL:CG1	1:A:270:LEU:HB2	2.50	0.42
4:D:159:GLN:HE21	4:D:159:GLN:HA	1.84	0.42
5:E:59:GLY:H	5:E:80:GLN:HE21	1.67	0.42
1:A:71:THR:O	1:A:75[A]:ARG:HG3	2.20	0.42
1:A:196:ASP:O	1:A:197:HIS:HB2	2.19	0.42
4:D:178:LEU:HB2	7:D:248:HOH:O	2.20	0.42
1:A:218:GLN:HE21	1:A:221:GLY:HA2	1.85	0.41
1:A:234:ARG:HE	1:A:242:GLN:HE21	1.68	0.41
1:A:226:GLN:H	1:A:226:GLN:HG2	1.67	0.41
5:E:239:LYS:HA	5:E:240:PRO:HD3	1.86	0.41
4:D:153:PHE:HB2	4:D:205:PHE:CE1	2.55	0.41
1:A:251:SER:C	1:A:253:GLU:H	2.24	0.40
5:E:180:VAL:HA	5:E:203:ARG:O	2.21	0.40
1:A:275:GLU:HA	1:A:276:PRO:HD3	1.90	0.40
3:C:6:ALA:HB3	3:C:9:PHE:CE1	2.56	0.40
5:E:139:GLU:OE1	5:E:252:ARG:NH1	2.54	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	281/276 (102%)	264 (94%)	15 (5%)	2 (1%)	22 18
2	B	100/100 (100%)	97 (97%)	2 (2%)	1 (1%)	15 11
3	C	9/11 (82%)	9 (100%)	0	0	100 100
4	D	209/200 (104%)	201 (96%)	6 (3%)	2 (1%)	15 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	242/242 (100%)	232 (96%)	8 (3%)	2 (1%)	19	15
All	All	841/829 (101%)	803 (96%)	31 (4%)	7 (1%)	22	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	198	ASP
2	B	47	GLU
1	A	198	GLU
1	A	252	GLY
4	D	197	SER
5	E	229[A]	GLU
5	E	229[B]	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	241/234 (103%)	230 (95%)	11 (5%)	27	26
2	B	97/95 (102%)	90 (93%)	7 (7%)	14	11
3	C	9/9 (100%)	9 (100%)	0	100	100
4	D	189/178 (106%)	169 (89%)	20 (11%)	6	4
5	E	212/210 (101%)	198 (93%)	14 (7%)	16	14
All	All	748/726 (103%)	696 (93%)	52 (7%)	15	12

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	17	ARG
1	A	108	ARG
1	A	121	LYS
1	A	145	ARG

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Mol	Chain	Res	Type
1	A	156	LEU
1	A	177	GLU
1	A	197	HIS
1	A	226	GLN
1	A	231	VAL
1	A	275	GLU
2	B	1	ILE
2	B	39	LEU
2	B	64	LEU
2	B	91	LYS
2	B	93[A]	VAL
2	B	93[B]	VAL
2	B	96	ASP
4	D	9[A]	GLU
4	D	9[B]	GLU
4	D	13	LEU
4	D	30	LEU
4	D	39	LEU
4	D	83	LEU
4	D	0	LYS
4	D	109	LEU
4	D	111	THR
4	D	123	GLN
4	D	149	SER
4	D	150	VAL
4	D	159	GLN
4	D	175	LYS
4	D	178	LEU
4	D	181	ARG
4	D	183	MET
4	D	196	LYS
4	D	197	SER
4	D	198	ASP
5	E	1	ASP
5	E	50	LEU
5	E	66	ARG
5	E	84	ASP
5	E	135	VAL
5	E	150	LYS
5	E	156	LEU
5	E	174	LYS
5	E	180	VAL

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Mol	Chain	Res	Type
5	E	182	THR
5	E	203	ARG
5	E	215	ARG
5	E	235	GLN
5	E	244	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	127	ASN
1	A	218	GLN
1	A	242	GLN
1	A	262	GLN
2	B	17	ASN
2	B	24	ASN
2	B	42	ASN
3	C	1	HIS
4	D	14	GLN
4	D	22	ASN
4	D	44	GLN
4	D	123	GLN
4	D	129	ASN
4	D	159	GLN
4	D	188	ASN
5	E	80	GLN
5	E	164	HIS
5	E	212	GLN
5	E	213	ASN
5	E	216	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	E	255	-	4,4,4	0.24	0	6,6,6	0.09	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	276/276 (100%)	0.17	9 (3%)	46	53	11, 26, 74, 91	7 (2%)
2	B	100/100 (100%)	0.62	7 (7%)	16	20	18, 43, 78, 87	0
3	C	11/11 (100%)	-0.34	0	100	100	13, 15, 18, 19	0
4	D	200/200 (100%)	0.13	7 (3%)	44	50	13, 23, 50, 59	1 (0%)
5	E	242/242 (100%)	0.13	6 (2%)	57	62	14, 26, 54, 87	11 (4%)
All	All	829/829 (100%)	0.19	29 (3%)	44	50	11, 26, 69, 91	19 (2%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	146	SER	5.1
1	A	196	ASP	4.8
2	B	46[A]	ILE	4.3
4	D	197	SER	4.1
5	E	254	ASP	4.1
4	D	195	ASN	3.9
5	E	0	MET	3.6
1	A	251	SER	3.3
4	D	147	ASP	3.1
2	B	0	MET	3.1
5	E	46	LEU	2.8
5	E	252	ARG	2.5
4	D	196	LYS	2.5
4	D	218	SER	2.5
1	A	17	ARG	2.4
1	A	270	LEU	2.3
5	E	228	SER	2.3
4	D	145	SER	2.3
2	B	48	LYS	2.3
5	E	229[A]	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	1	ILE	2.2
1	A	90	ALA	2.2
2	B	86	THR	2.2
2	B	94	LYS	2.2
2	B	92	ILE	2.1
1	A	221	GLY	2.1
1	A	252	GLY	2.1
1	A	16	GLY	2.0
1	A	195	SER	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	E	255	5/5	0.93	0.14	59,59,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.