



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:16 am GMT

PDB ID : 4JFF  
Title : Preservation of peptide specificity during TCR-MHC contact dominated affinity enhancement of a melanoma-specific TCR  
Authors : Rizkallah, P.J.; Cole, D.K.; Madura, F.; Sewell, A.K.  
Deposited on : 2013-02-28  
Resolution : 2.43 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

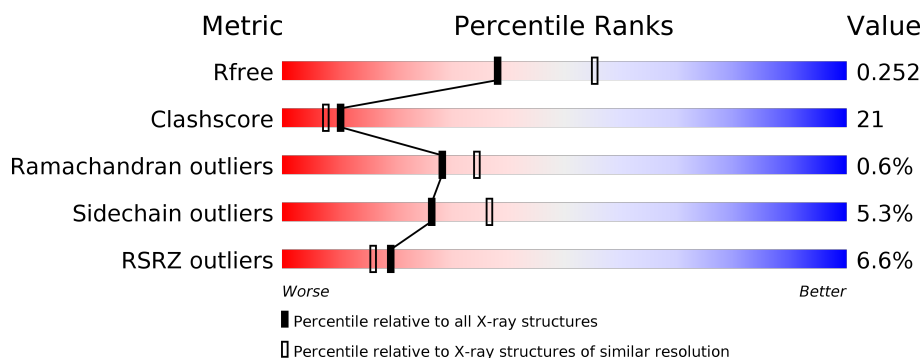
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 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))
$R_{free}$	100719	1152 (2.46-2.42)
Clashscore	112137	1224 (2.46-2.42)
Ramachandran outliers	110173	1217 (2.46-2.42)
Sidechain outliers	110143	1217 (2.46-2.42)
RSRZ outliers	101464	1158 (2.46-2.42)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>15%</div> <div>64% 32%</div> </div>
2	B	100	<div> <div>3%</div> <div>71% 26%</div> </div>
3	C	10	<div> <div>60% 40%</div> </div>
4	D	197	<div> <div>5%</div> <div>64% 30% 5%</div> </div>
5	E	245	<div> <div>%</div> <div>74% 23%</div> </div>

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
6	EPE	A	301	-	-	-	X
7	SO4	E	302	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6874 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, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

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 Melanoma motif.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			69	45	10	14			

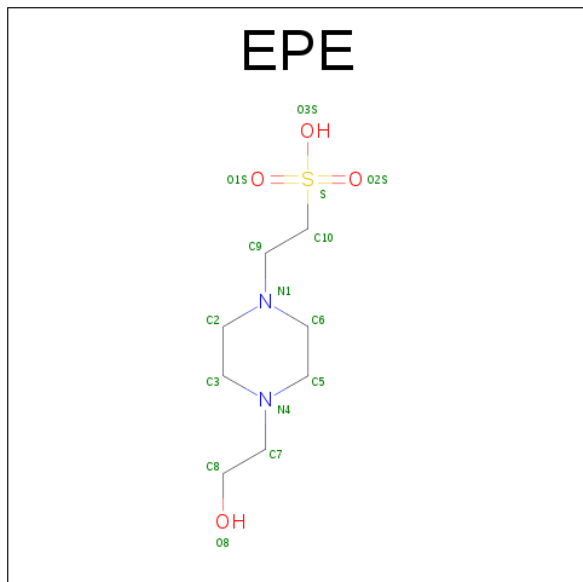
- Molecule 4 is a protein called High Affinity TCR Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	197	Total	C	N	O	S	0	0	0
			1536	956	256	316	8			

- Molecule 5 is a protein called High Affinity TCR Beta Chain.

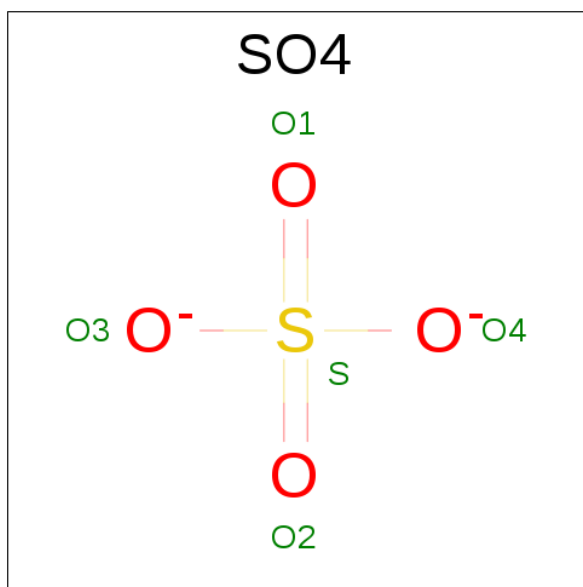
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C	N	O	S	0	1	0
			1954	1241	337	369	7			

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
6	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0

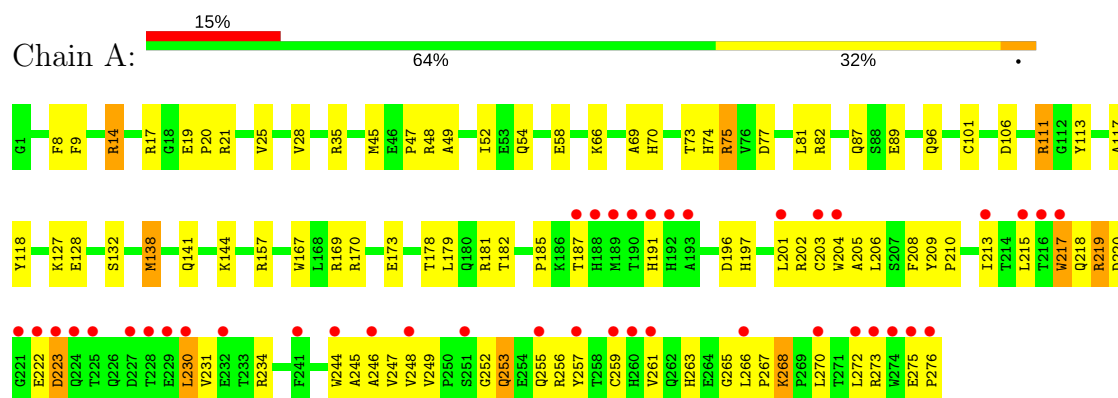
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	39	Total O 39 39	0	0
8	B	20	Total O 20 20	0	0
8	C	1	Total O 1 1	0	0
8	D	45	Total O 45 45	0	0
8	E	54	Total O 54 54	0	0

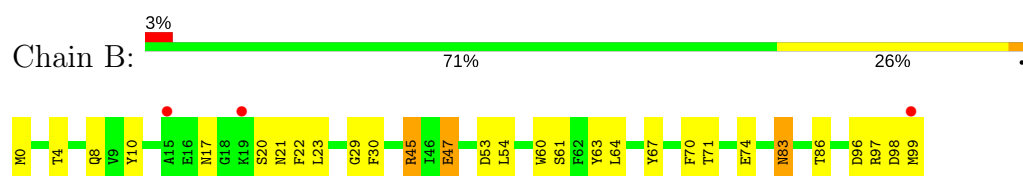
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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, A-2 alpha chain



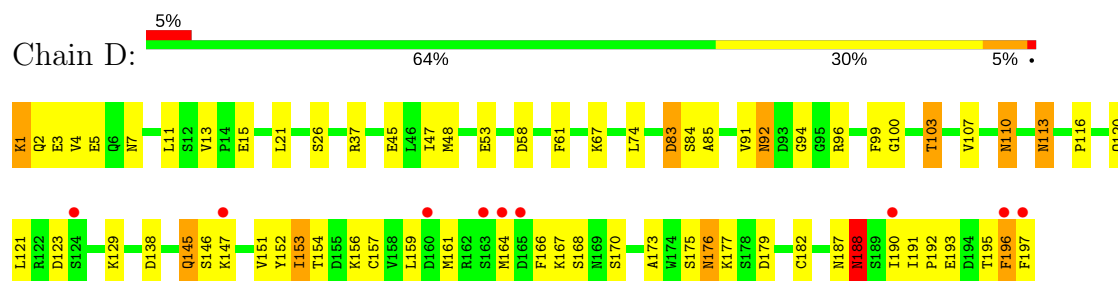
- Molecule 2: Beta-2-microglobulin



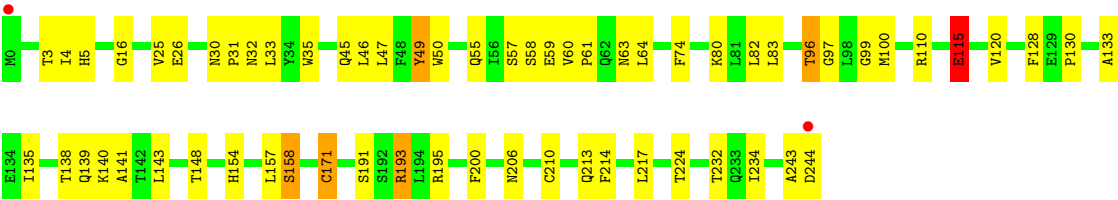
- Molecule 3: Melanoma motif



- Molecule 4: High Affinity TCR Alpha Chain



- Molecule 5: High Affinity TCR Beta Chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.44Å 121.44Å 82.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.13 – 2.43 68.13 – 2.43	Depositor EDS
% Data completeness (in resolution range)	100.0 (68.13-2.43) 100.0 (68.13-2.43)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.210 , 0.263 0.204 , 0.252	Depositor DCC
$R_{free}$ test set	2278 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6874	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: EPE, 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	1.03	1/2320 (0.0%)	0.57	1/3149 (0.0%)
2	B	0.92	1/860 (0.1%)	0.59	0/1162
3	C	1.05	0/68	0.76	0/90
4	D	1.07	3/1568 (0.2%)	0.62	0/2123
5	E	1.11	3/2014 (0.1%)	0.63	0/2747
All	All	1.05	8/6830 (0.1%)	0.60	1/9271 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	CYS	CB-SG	-19.72	1.48	1.82
5	E	210	CYS	CB-SG	-9.59	1.66	1.82
5	E	115	GLU	CG-CD	7.67	1.63	1.51
5	E	158	SER	CB-OG	-6.52	1.33	1.42
2	B	47	GLU	CB-CG	6.35	1.64	1.52
4	D	83	ASP	CB-CG	-5.88	1.39	1.51
4	D	91	VAL	CB-CG1	-5.57	1.41	1.52
4	D	5	GLU	CG-CD	5.43	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	CYS	CB-CA-C	-5.50	99.41	110.40

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	2254	0	2103	109	0
2	B	837	0	803	35	0
3	C	69	0	79	6	0
4	D	1536	0	1448	77	0
5	E	1954	0	1854	71	0
6	A	15	0	18	1	0
6	E	15	0	17	3	0
7	A	15	0	0	1	0
7	D	5	0	0	0	0
7	E	15	0	0	0	0
8	A	39	0	0	0	0
8	B	20	0	0	1	0
8	C	1	0	0	0	0
8	D	45	0	0	4	0
8	E	54	0	0	0	0
All	All	6874	0	6322	271	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 (271) 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:266:LEU:HD23	1:A:270:LEU:CD2	1.56	1.35
1:A:185:PRO:HD2	1:A:266:LEU:HD11	1.25	1.11
1:A:266:LEU:CD2	1:A:270:LEU:HD23	1.85	1.05
5:E:135:ILE:HD11	5:E:141:ALA:HB2	1.40	1.04
1:A:266:LEU:HD23	1:A:270:LEU:HD23	1.03	1.02
1:A:261:VAL:HG22	1:A:270:LEU:HB2	1.41	1.01
1:A:266:LEU:HD23	1:A:270:LEU:HD21	1.51	0.93
1:A:261:VAL:CG2	1:A:270:LEU:HB2	1.99	0.91
5:E:58:SER:N	6:E:301:EPE:O1S	2.02	0.90
1:A:230:LEU:O	1:A:230:LEU:HD22	1.72	0.90
1:A:253:GLN:OE1	1:A:253:GLN:O	1.92	0.87
5:E:63:ASN:ND2	5:E:82:LEU:HD13	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:135:ILE:CD1	5:E:141:ALA:HB2	2.07	0.85
4:D:195:THR:HG21	5:E:133:ALA:HB1	1.60	0.83
2:B:45:ARG:CG	2:B:45:ARG:HH11	1.91	0.82
2:B:4:THR:HG22	2:B:86:THR:HB	1.63	0.79
5:E:130:PRO:HD3	5:E:143:LEU:CD2	2.12	0.79
1:A:77:ASP:OD1	3:C:9:THR:HG23	1.83	0.79
1:A:185:PRO:HD2	1:A:266:LEU:CD1	2.10	0.78
2:B:63:TYR:O	2:B:64:LEU:HD12	1.85	0.77
4:D:7:ASN:O	4:D:103:THR:HB	1.83	0.76
2:B:54:LEU:CD1	2:B:64:LEU:HD11	2.15	0.76
2:B:45:ARG:HG3	2:B:45:ARG:HH11	1.52	0.75
1:A:249:VAL:HG11	1:A:257:TYR:CZ	2.22	0.75
1:A:138:MET:CE	1:A:138:MET:HA	2.16	0.74
1:A:230:LEU:HD13	1:A:230:LEU:H	1.53	0.74
1:A:266:LEU:CD2	1:A:270:LEU:CD2	2.51	0.73
4:D:195:THR:HG21	5:E:133:ALA:CB	2.19	0.73
2:B:63:TYR:C	2:B:64:LEU:HD12	2.08	0.73
4:D:153:ILE:HD13	4:D:153:ILE:C	2.08	0.73
1:A:111:ARG:HD2	1:A:113:TYR:CE2	2.23	0.73
1:A:111:ARG:HD2	1:A:113:TYR:CZ	2.23	0.72
4:D:37:ARG:NH2	4:D:45:GLU:OE2	2.20	0.72
5:E:3:THR:CG2	5:E:5:HIS:CE1	2.72	0.72
1:A:138:MET:HE2	1:A:138:MET:HA	1.72	0.70
4:D:1:LYS:NZ	5:E:45:GLN:HE22	1.89	0.70
2:B:54:LEU:HD12	2:B:64:LEU:HD11	1.73	0.70
1:A:73:THR:CG2	5:E:97:GLY:HA2	2.20	0.70
1:A:215:LEU:HD11	1:A:259:CYS:SG	2.31	0.69
1:A:45:MET:CE	3:C:2:LEU:HD11	2.21	0.69
1:A:49:ALA:O	1:A:52:ILE:HG22	1.92	0.69
5:E:31:PRO:HG2	5:E:33:LEU:HD11	1.73	0.69
5:E:32:ASN:O	5:E:33:LEU:HD12	1.92	0.69
5:E:110:ARG:HD3	5:E:154[B]:HIS:CD2	2.28	0.69
5:E:3:THR:HG21	5:E:5:HIS:CE1	2.28	0.69
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.28	0.68
1:A:196:ASP:O	1:A:197:HIS:HB3	1.92	0.68
1:A:73:THR:HG21	5:E:97:GLY:HA2	1.74	0.68
5:E:135:ILE:HD11	5:E:141:ALA:CB	2.22	0.67
4:D:153:ILE:HD13	4:D:153:ILE:O	1.94	0.67
5:E:32:ASN:C	5:E:33:LEU:HD12	2.14	0.67
1:A:204:TRP:HB3	1:A:206:LEU:HD21	1.77	0.67
4:D:47:ILE:HG22	4:D:48:MET:HG3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:190:ILE:HG23	4:D:190:ILE:O	1.95	0.66
4:D:1:LYS:HZ2	5:E:45:GLN:HE22	1.43	0.66
4:D:164:MET:O	4:D:164:MET:HG2	1.96	0.65
5:E:130:PRO:HG3	5:E:143:LEU:HD23	1.78	0.65
4:D:4:VAL:HG13	4:D:100:GLY:HA2	1.79	0.64
4:D:48:MET:HE3	4:D:61:PHE:C	2.17	0.64
1:A:197:HIS:O	1:A:197:HIS:CG	2.50	0.64
5:E:30:ASN:O	5:E:96:THR:HB	1.97	0.64
1:A:249:VAL:CG1	1:A:257:TYR:CZ	2.80	0.64
5:E:63:ASN:O	5:E:64:LEU:HD12	1.97	0.64
1:A:231:VAL:HG11	2:B:8:GLN:OE1	1.98	0.64
5:E:138:THR:HG21	5:E:140:LYS:HE3	1.80	0.63
1:A:138:MET:HE2	1:A:141:GLN:HG3	1.80	0.63
5:E:157:LEU:HD23	5:E:158:SER:N	2.14	0.62
4:D:48:MET:HE3	4:D:61:PHE:O	1.99	0.62
5:E:33:LEU:HD23	5:E:74:PHE:HB2	1.81	0.62
4:D:4:VAL:HG12	8:D:314:HOH:O	1.98	0.62
4:D:110:ASN:C	4:D:110:ASN:HD22	2.04	0.61
4:D:92:ASN:HD22	4:D:92:ASN:C	2.04	0.61
1:A:87:GLN:OE1	1:A:118:TYR:OH	2.08	0.60
1:A:263:HIS:HB3	1:A:266:LEU:HD13	1.83	0.60
4:D:116:PRO:HB2	4:D:192:PRO:HB3	1.84	0.60
1:A:219:ARG:O	1:A:220:ASP:OD2	2.20	0.60
4:D:161:MET:HE1	5:E:195:ARG:HD3	1.83	0.60
4:D:15:GLU:OE2	4:D:167:LYS:NZ	2.34	0.59
1:A:202:ARG:HH22	2:B:99:MET:HE1	1.67	0.59
4:D:196:PHE:O	4:D:197:PHE:C	2.41	0.59
5:E:115:GLU:H	5:E:115:GLU:CD	2.06	0.59
1:A:266:LEU:N	1:A:266:LEU:HD12	2.18	0.59
1:A:217:TRP:CH2	1:A:245:ALA:O	2.56	0.58
3:C:7:ILE:C	3:C:8:LEU:HD23	2.25	0.57
4:D:53:GLU:OE2	4:D:67:LYS:N	2.36	0.57
1:A:219:ARG:HD3	1:A:219:ARG:O	2.05	0.57
5:E:3:THR:CG2	5:E:4:ILE:N	2.67	0.57
2:B:98:ASP:O	2:B:99:MET:HG2	2.04	0.57
4:D:113:ASN:H	4:D:113:ASN:ND2	2.03	0.57
2:B:4:THR:HG21	8:B:414:HOH:O	2.05	0.56
5:E:120:VAL:HG21	5:E:217:LEU:HD21	1.87	0.56
1:A:178:THR:O	1:A:181:ARG:HG2	2.06	0.56
1:A:187:THR:OG1	1:A:272:LEU:HD11	2.06	0.56
1:A:182:THR:HG23	1:A:182:THR:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:146:SER:CB	4:D:151:VAL:CG2	2.83	0.56
1:A:202:ARG:HD3	1:A:246:ALA:HB2	1.87	0.56
5:E:224:THR:O	5:E:224:THR:HG22	2.06	0.56
5:E:3:THR:HG23	5:E:5:HIS:CE1	2.40	0.55
1:A:20:PRO:CD	1:A:75:ARG:HD3	2.36	0.55
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.42	0.55
4:D:92:ASN:HD22	4:D:94:GLY:H	1.54	0.55
1:A:206:LEU:HD22	1:A:206:LEU:N	2.21	0.55
1:A:231:VAL:CG1	2:B:8:GLN:OE1	2.55	0.55
4:D:1:LYS:HG2	8:D:314:HOH:O	2.06	0.55
4:D:92:ASN:ND2	4:D:94:GLY:H	2.05	0.55
1:A:202:ARG:NH1	2:B:99:MET:HE2	2.21	0.55
1:A:191:HIS:HB3	1:A:276:PRO:HG2	1.89	0.54
5:E:16:GLY:HA2	5:E:80:LYS:HG3	1.90	0.54
4:D:152:TYR:O	4:D:173:ALA:HA	2.06	0.54
5:E:138:THR:HG22	5:E:139:GLN:H	1.73	0.54
5:E:35:TRP:CD1	5:E:74:PHE:CE2	2.96	0.54
1:A:14:ARG:HD3	1:A:19:GLU:O	2.08	0.54
1:A:215:LEU:CD1	1:A:259:CYS:SG	2.95	0.54
4:D:1:LYS:HG3	4:D:3:GLU:H	1.73	0.54
5:E:200:PHE:O	5:E:206:ASN:ND2	2.35	0.54
1:A:77:ASP:OD1	3:C:9:THR:CG2	2.56	0.54
1:A:202:ARG:HH12	2:B:99:MET:HE2	1.72	0.53
4:D:176:ASN:HD22	4:D:176:ASN:N	2.05	0.53
4:D:4:VAL:HG11	4:D:99:PHE:C	2.29	0.53
4:D:113:ASN:HD22	4:D:113:ASN:H	1.56	0.53
1:A:203:CYS:SG	1:A:215:LEU:HD11	2.48	0.53
5:E:33:LEU:CD1	5:E:33:LEU:N	2.71	0.53
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.90	0.53
1:A:265:GLY:C	1:A:266:LEU:HD12	2.29	0.53
5:E:224:THR:O	5:E:224:THR:CG2	2.57	0.53
4:D:156:LYS:HA	4:D:170:SER:O	2.09	0.52
1:A:21:ARG:NH1	7:A:302:SO4:O3	2.43	0.52
4:D:1:LYS:HG3	4:D:2:GLN:H	1.74	0.52
5:E:30:ASN:N	5:E:31:PRO:CD	2.73	0.52
4:D:48:MET:CE	4:D:61:PHE:O	2.57	0.52
1:A:204:TRP:HB3	1:A:206:LEU:CD2	2.40	0.52
2:B:30:PHE:HZ	2:B:64:LEU:HD13	1.74	0.52
1:A:230:LEU:C	1:A:230:LEU:HD22	2.30	0.52
1:A:66:LYS:O	1:A:70:HIS:HD2	1.93	0.52
4:D:188:ASN:O	4:D:188:ASN:ND2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:PHE:CZ	1:A:213:ILE:HG21	2.44	0.52
5:E:130:PRO:HD3	5:E:143:LEU:HD23	1.90	0.52
5:E:58:SER:HB2	6:E:301:EPE:O1S	2.10	0.52
5:E:60:VAL:O	5:E:60:VAL:HG23	2.10	0.51
2:B:98:ASP:OD1	2:B:99:MET:N	2.42	0.51
2:B:98:ASP:O	2:B:99:MET:CG	2.59	0.51
5:E:135:ILE:O	5:E:138:THR:O	2.28	0.51
4:D:161:MET:HE3	4:D:166:PHE:CD2	2.46	0.51
4:D:1:LYS:HG3	4:D:2:GLN:N	2.26	0.51
1:A:54:GLN:HA	1:A:54:GLN:HE21	1.76	0.51
4:D:191:ILE:O	4:D:191:ILE:HD12	2.11	0.51
4:D:176:ASN:HD22	4:D:176:ASN:H	1.57	0.51
1:A:205:ALA:C	1:A:206:LEU:HD22	2.31	0.51
1:A:20:PRO:HD3	1:A:75:ARG:HD3	1.93	0.51
5:E:130:PRO:HD3	5:E:143:LEU:HD22	1.90	0.51
1:A:202:ARG:HH22	2:B:99:MET:CE	2.24	0.50
4:D:123:ASP:HB3	5:E:128:PHE:CD2	2.46	0.50
5:E:3:THR:HG21	5:E:5:HIS:HE1	1.74	0.50
1:A:249:VAL:HG11	1:A:257:TYR:CE1	2.47	0.50
1:A:20:PRO:HG2	1:A:75:ARG:HG2	1.93	0.50
5:E:63:ASN:ND2	5:E:80:LYS:O	2.29	0.50
1:A:230:LEU:H	1:A:230:LEU:CD1	2.22	0.50
5:E:130:PRO:CG	5:E:143:LEU:HD23	2.42	0.50
5:E:110:ARG:HD3	5:E:154[B]:HIS:NE2	2.25	0.50
5:E:243:ALA:O	5:E:244:ASP:C	2.51	0.49
5:E:234:ILE:N	5:E:234:ILE:HD12	2.27	0.49
1:A:222:GLU:O	1:A:223:ASP:CB	2.61	0.49
1:A:82:ARG:CZ	1:A:89:GLU:OE2	2.61	0.49
5:E:193:ARG:N	5:E:193:ARG:HD2	2.28	0.49
1:A:169:ARG:O	1:A:173:GLU:HG3	2.13	0.49
1:A:219:ARG:C	1:A:219:ARG:HD3	2.32	0.49
1:A:217:TRP:CE3	1:A:247:VAL:HG13	2.48	0.49
4:D:159:LEU:HD12	4:D:159:LEU:O	2.13	0.49
5:E:99:GLY:O	5:E:100:MET:HE2	2.13	0.49
1:A:244:TRP:NE1	2:B:99:MET:HA	2.27	0.48
4:D:188:ASN:C	4:D:188:ASN:HD22	2.16	0.48
2:B:4:THR:HG22	2:B:86:THR:CB	2.39	0.48
4:D:191:ILE:CD1	4:D:191:ILE:O	2.62	0.48
2:B:45:ARG:HG2	2:B:45:ARG:HH11	1.71	0.48
5:E:32:ASN:C	5:E:33:LEU:CD1	2.81	0.48
4:D:96:ARG:HD2	5:E:46:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLU:H	1:A:58:GLU:CD	2.17	0.48
2:B:17:ASN:ND2	2:B:74:GLU:HG3	2.28	0.48
4:D:121:LEU:HD12	4:D:121:LEU:N	2.29	0.48
5:E:63:ASN:ND2	5:E:82:LEU:CD1	2.69	0.48
1:A:218:GLN:HG2	1:A:222:GLU:CD	2.35	0.47
4:D:146:SER:HB3	4:D:151:VAL:CG2	2.44	0.47
4:D:4:VAL:HG13	4:D:100:GLY:CA	2.44	0.47
2:B:45:ARG:NH1	2:B:45:ARG:CG	2.61	0.47
4:D:175:SER:OG	4:D:177:LYS:HG2	2.14	0.47
4:D:179:ASP:OD2	4:D:179:ASP:C	2.51	0.47
1:A:217:TRP:CZ3	1:A:245:ALA:C	2.88	0.47
4:D:159:LEU:CD1	4:D:168:SER:HB3	2.45	0.47
5:E:58:SER:CB	6:E:301:EPE:O1S	2.63	0.47
1:A:45:MET:HE1	3:C:2:LEU:HD11	1.94	0.47
1:A:219:ARG:C	1:A:219:ARG:CD	2.84	0.46
4:D:146:SER:HB3	4:D:151:VAL:HG22	1.97	0.46
1:A:266:LEU:N	1:A:266:LEU:CD1	2.78	0.46
4:D:48:MET:HE1	4:D:58:ASP:N	2.30	0.46
4:D:193:GLU:O	4:D:193:GLU:HG3	2.16	0.46
1:A:47:PRO:O	1:A:48:ARG:HD2	2.16	0.46
1:A:106:ASP:O	6:A:301:EPE:O2S	2.33	0.45
4:D:4:VAL:CG1	8:D:314:HOH:O	2.62	0.45
2:B:98:ASP:C	2:B:99:MET:HG2	2.37	0.45
1:A:54:GLN:HA	1:A:54:GLN:NE2	2.31	0.45
1:A:234:ARG:HD2	2:B:10:TYR:CE2	2.51	0.45
4:D:159:LEU:HB3	5:E:171:CYS:HB3	1.99	0.45
1:A:111:ARG:CD	1:A:113:TYR:CZ	2.98	0.45
4:D:153:ILE:CD1	4:D:154:THR:O	2.65	0.45
1:A:167:TRP:CE3	1:A:170:ARG:HD3	2.52	0.45
1:A:222:GLU:OE1	1:A:222:GLU:N	2.35	0.45
5:E:59:GLU:HG3	5:E:61:PRO:HD3	1.98	0.45
1:A:201:LEU:N	1:A:201:LEU:HD12	2.32	0.45
5:E:59:GLU:OE2	5:E:60:VAL:N	2.49	0.45
1:A:69:ALA:O	1:A:73:THR:HG23	2.17	0.44
2:B:96:ASP:O	2:B:98:ASP:O	2.36	0.44
4:D:13:VAL:CG2	4:D:107:VAL:HG22	2.48	0.44
1:A:222:GLU:O	1:A:223:ASP:HB3	2.18	0.44
1:A:255:GLN:HG2	1:A:275:GLU:OE1	2.17	0.44
1:A:275:GLU:N	1:A:275:GLU:CD	2.71	0.44
2:B:20:SER:HA	2:B:71:THR:HG22	1.99	0.44
5:E:130:PRO:CD	5:E:143:LEU:CD2	2.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:3:THR:HG22	5:E:4:ILE:N	2.32	0.44
1:A:127:LYS:HD2	1:A:132:SER:HB2	2.00	0.44
4:D:146:SER:CB	4:D:151:VAL:HG21	2.48	0.43
5:E:25:VAL:HG22	5:E:26:GLU:N	2.32	0.43
4:D:21:LEU:HD12	4:D:74:LEU:HD23	1.99	0.43
5:E:130:PRO:CD	5:E:143:LEU:HD23	2.47	0.43
5:E:49:TYR:HB3	5:E:57:SER:HB3	2.00	0.43
1:A:217:TRP:HZ3	1:A:245:ALA:C	2.21	0.43
2:B:23:LEU:O	2:B:67:TYR:HA	2.19	0.43
1:A:267:PRO:C	1:A:268:LYS:HE2	2.39	0.43
1:A:8:PHE:HB2	1:A:25:VAL:HG12	2.00	0.43
5:E:50:TRP:HE1	5:E:55:GLN:HE21	1.65	0.43
4:D:37:ARG:HB2	4:D:47:ILE:HD11	2.00	0.42
1:A:270:LEU:N	1:A:270:LEU:HD22	2.34	0.42
1:A:82:ARG:NH1	1:A:89:GLU:OE2	2.52	0.42
2:B:54:LEU:HD13	2:B:64:LEU:HD11	1.99	0.42
1:A:248:VAL:C	1:A:249:VAL:HG13	2.40	0.42
2:B:17:ASN:ND2	2:B:74:GLU:CG	2.83	0.42
1:A:111:ARG:CZ	1:A:128:GLU:OE2	2.68	0.42
1:A:217:TRP:HZ3	1:A:246:ALA:N	2.18	0.42
5:E:83:LEU:HD21	5:E:115:GLU:HG3	2.02	0.42
1:A:209:TYR:HA	1:A:210:PRO:O	2.20	0.42
2:B:29:GLY:HA2	2:B:61:SER:HB2	2.02	0.42
2:B:83:ASN:HD22	2:B:83:ASN:HA	1.64	0.42
4:D:138:ASP:N	4:D:138:ASP:OD2	2.48	0.41
3:C:7:ILE:O	3:C:8:LEU:HD23	2.19	0.41
4:D:159:LEU:HB3	5:E:171:CYS:CB	2.50	0.41
2:B:21:ASN:OD1	2:B:22:PHE:N	2.44	0.41
4:D:153:ILE:HD13	4:D:154:THR:O	2.19	0.41
4:D:84:SER:O	4:D:85:ALA:HB2	2.20	0.41
1:A:9:PHE:O	1:A:96:GLN:HA	2.21	0.41
4:D:159:LEU:HD11	4:D:168:SER:HB3	2.01	0.41
4:D:48:MET:HE2	4:D:58:ASP:HB3	2.01	0.41
1:A:219:ARG:HA	1:A:256:ARG:O	2.20	0.41
1:A:82:ARG:HA	1:A:87:GLN:HG2	2.01	0.41
4:D:1:LYS:HE3	8:D:325:HOH:O	2.20	0.41
4:D:92:ASN:C	4:D:92:ASN:ND2	2.73	0.41
5:E:214:PHE:O	5:E:232:THR:HG23	2.21	0.41
1:A:138:MET:CE	1:A:141:GLN:HG3	2.49	0.41
1:A:182:THR:O	1:A:182:THR:CG2	2.68	0.41
4:D:129:LYS:HE2	5:E:148:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:187:ASN:O	4:D:188:ASN:CB	2.69	0.41
4:D:3:GLU:HA	4:D:26:SER:OG	2.20	0.41
4:D:83:ASP:OD2	4:D:107:VAL:HG21	2.21	0.41
1:A:217:TRP:HH2	1:A:245:ALA:O	2.00	0.41
4:D:145:GLN:HE21	4:D:145:GLN:HA	1.84	0.41
4:D:154:THR:HG21	5:E:191:SER:OG	2.21	0.41
4:D:120:GLN:HB2	4:D:182:CYS:SG	2.61	0.40
1:A:82:ARG:HA	1:A:87:GLN:CG	2.51	0.40
5:E:16:GLY:HA2	5:E:80:LYS:CG	2.51	0.40
5:E:63:ASN:C	5:E:64:LEU:HD12	2.41	0.40
1:A:138:MET:HE3	1:A:138:MET:HA	2.00	0.40
1:A:35:ARG:HD2	2:B:53:ASP:OD2	2.22	0.40
4:D:113:ASN:N	4:D:113:ASN:ND2	2.63	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	274/276 (99%)	253 (92%)	18 (7%)	3 (1%)	17	18
2	B	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
3	C	8/10 (80%)	8 (100%)	0	0	100	100
4	D	195/197 (99%)	183 (94%)	10 (5%)	2 (1%)	18	20
5	E	244/245 (100%)	237 (97%)	7 (3%)	0	100	100
All	All	819/828 (99%)	775 (95%)	39 (5%)	5 (1%)	28	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	GLY

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Mol	Chain	Res	Type
4	D	188	ASN
1	A	223	ASP
1	A	273	ARG
4	D	196	PHE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/232 (100%)	219 (94%)	13 (6%)	25	33
2	B	95/95 (100%)	89 (94%)	6 (6%)	21	28
3	C	7/7 (100%)	7 (100%)	0	100	100
4	D	175/175 (100%)	163 (93%)	12 (7%)	18	23
5	E	212/211 (100%)	205 (97%)	7 (3%)	43	58
All	All	721/720 (100%)	683 (95%)	38 (5%)	26	37

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	17	ARG
1	A	74	HIS
1	A	75	ARG
1	A	111	ARG
1	A	138	MET
1	A	144	LYS
1	A	157	ARG
1	A	217	TRP
1	A	219	ARG
1	A	230	LEU
1	A	253	GLN
1	A	268	LYS
2	B	0	MET
2	B	45	ARG

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Mol	Chain	Res	Type
2	B	47	GLU
2	B	70	PHE
2	B	83	ASN
2	B	97	ARG
4	D	1	LYS
4	D	11	LEU
4	D	92	ASN
4	D	103	THR
4	D	110	ASN
4	D	113	ASN
4	D	145	GLN
4	D	147	LYS
4	D	153	ILE
4	D	157	CYS
4	D	176	ASN
4	D	188	ASN
5	E	47	LEU
5	E	49	TYR
5	E	96	THR
5	E	115	GLU
5	E	171	CYS
5	E	193	ARG
5	E	213	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	70	HIS
1	A	74	HIS
1	A	86	ASN
1	A	93	HIS
1	A	174	ASN
1	A	180	GLN
1	A	262	GLN
2	B	17	ASN
2	B	83	ASN
4	D	2	GLN
4	D	38	GLN
4	D	92	ASN
4	D	110	ASN
4	D	113	ASN

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Mol	Chain	Res	Type
4	D	145	GLN
4	D	176	ASN
4	D	184	ASN
4	D	188	ASN
5	E	2	GLN
5	E	5	HIS
5	E	38	GLN
5	E	45	GLN
5	E	55	GLN
5	E	70	GLN
5	E	119	ASN
5	E	139	GLN
5	E	180	GLN
5	E	184	ASN
5	E	207	HIS

### 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](#)

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
6	EPE	A	301	-	15,15,15	1.26	1 (6%)	18,20,20	1.47	3 (16%)
7	SO4	A	302	-	4,4,4	0.34	0	6,6,6	0.18	0
7	SO4	A	303	-	4,4,4	0.28	0	6,6,6	0.12	0
7	SO4	A	304	-	4,4,4	0.50	0	6,6,6	0.21	0
7	SO4	D	201	-	4,4,4	0.44	0	6,6,6	0.11	0
6	EPE	E	301	-	15,15,15	0.75	1 (6%)	18,20,20	1.33	2 (11%)
7	SO4	E	302	-	4,4,4	0.21	0	6,6,6	0.07	0
7	SO4	E	303	-	4,4,4	0.24	0	6,6,6	0.06	0
7	SO4	E	304	-	4,4,4	0.33	0	6,6,6	0.08	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
6	EPE	A	301	-	-	0/9/19/19	0/1/1/1
7	SO4	A	302	-	-	0/0/0/0	0/0/0/0
7	SO4	A	303	-	-	0/0/0/0	0/0/0/0
7	SO4	A	304	-	-	0/0/0/0	0/0/0/0
7	SO4	D	201	-	-	0/0/0/0	0/0/0/0
6	EPE	E	301	-	-	0/9/19/19	0/1/1/1
7	SO4	E	302	-	-	0/0/0/0	0/0/0/0
7	SO4	E	303	-	-	0/0/0/0	0/0/0/0
7	SO4	E	304	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	301	EPE	C10-S	2.17	1.80	1.77
6	A	301	EPE	C10-S	4.17	1.83	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	301	EPE	O3S-S-C10	2.32	108.91	106.06
6	E	301	EPE	O2S-S-C10	2.71	109.12	106.79
6	A	301	EPE	O2S-S-C10	3.22	109.56	106.79
6	E	301	EPE	O3S-S-C10	3.56	110.44	106.06
6	A	301	EPE	O1S-S-C10	3.70	109.97	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	EPE	1	0
7	A	302	SO4	1	0
6	E	301	EPE	3	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	276/276 (100%)	0.55	41 (14%) 3 1	23, 49, 139, 170	0
2	B	100/100 (100%)	0.23	3 (3%) 51 46	27, 56, 117, 137	0
3	C	10/10 (100%)	0.00	0 100 100	24, 26, 35, 35	0
4	D	197/197 (100%)	0.16	9 (4%) 33 31	21, 43, 102, 146	0
5	E	245/245 (100%)	-0.14	2 (0%) 86 87	23, 41, 82, 114	0
All	All	828/828 (100%)	0.21	55 (6%) 19 16	21, 45, 117, 170	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	TYR	6.4
1	A	276	PRO	6.0
1	A	215	LEU	5.6
1	A	272	LEU	4.7
5	E	244	ASP	4.6
4	D	190	ILE	4.6
1	A	204	TRP	4.5
4	D	164	MET	4.4
1	A	274	TRP	4.3
1	A	203	CYS	4.3
1	A	261	VAL	3.9
1	A	225	THR	3.9
4	D	163	SER	3.8
1	A	217	TRP	3.8
5	E	0	MET	3.6
1	A	275	GLU	3.5
4	D	124	SER	3.5
1	A	191	HIS	3.4
1	A	228	THR	3.4
1	A	216	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	229	GLU	3.3
1	A	259	CYS	3.3
1	A	246	ALA	3.2
2	B	15	ALA	3.2
2	B	99	MET	3.2
1	A	213	ILE	3.1
1	A	223	ASP	3.1
1	A	201	LEU	3.0
1	A	222	GLU	2.9
1	A	227	ASP	2.9
1	A	255	GLN	2.9
1	A	188	HIS	2.8
1	A	230	LEU	2.8
1	A	251	SER	2.8
1	A	187	THR	2.8
1	A	266	LEU	2.8
1	A	270	LEU	2.8
1	A	273	ARG	2.7
4	D	197	PHE	2.7
4	D	147	LYS	2.5
2	B	19	LYS	2.5
1	A	241	PHE	2.5
1	A	248	VAL	2.4
1	A	260	HIS	2.4
4	D	160	ASP	2.4
1	A	193	ALA	2.4
1	A	192	HIS	2.3
1	A	244	TRP	2.2
1	A	190	THR	2.2
1	A	189	MET	2.2
4	D	165	ASP	2.1
1	A	232	GLU	2.1
1	A	224	GLN	2.0
1	A	221	GLY	2.0
4	D	196	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	EPE	A	301	15/15	0.53	0.25	5.16	90,100,100,100	0
7	SO4	E	302	5/5	0.92	0.20	2.61	99,100,100,100	0
7	SO4	A	303	5/5	0.97	0.23	1.52	67,72,74,77	0
7	SO4	E	304	5/5	0.84	0.20	1.08	100,100,100,100	0
6	EPE	E	301	15/15	0.95	0.20	0.72	54,80,91,91	0
7	SO4	A	304	5/5	0.94	0.13	-1.45	50,54,60,62	0
7	SO4	E	303	5/5	0.84	0.16	-	94,96,98,99	0
7	SO4	A	302	5/5	0.93	0.10	-	70,71,74,76	0
7	SO4	D	201	5/5	0.94	0.18	-	68,73,75,75	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.