Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:10 AM GMT

PDB ID	:	2W65
Title	:	ANTI CITRULLINATED COLLAGEN TYPE 2 ANTIBODY ACC4 IN COMPLEX WITH A CITRULLINATED PEPTIDE
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Deposited on	:	2008-12-17
Resolution	:	2.21 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:

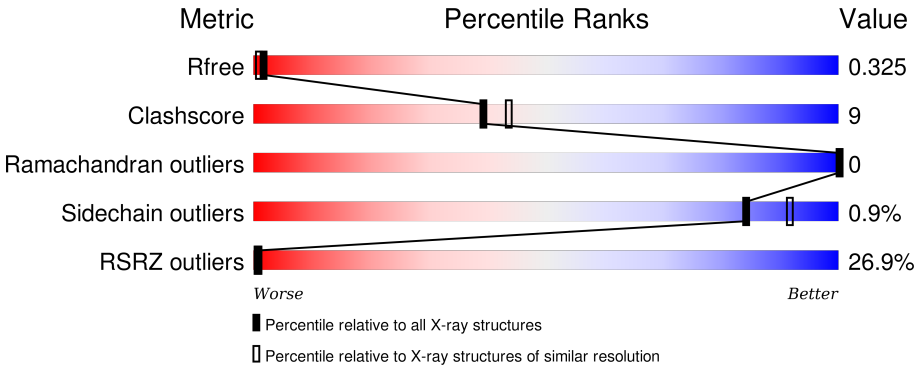
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.21 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	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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	218	19% 83% 14%
1	C	218	29% 84% 12%
2	B	217	28% 87% 13%
2	D	217	30% 76% 24%
3	E	9	22% 67% 22% 11%

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Mol	Chain	Length	Quality of chain
3	F	9	78% 22%

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	CIR	E	2	X	-	-	-
3	HYP	E	8	X	-	-	-
3	CIR	F	2	X	-	-	-
3	HYP	F	8	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6893 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 ANTI-CITRULLINATED COLLAGEN TYPE II FAB ACC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1603	1026	257	314	6			
1	C	211	Total	C	N	O	S	0	0	0
			1599	1024	256	313	6			

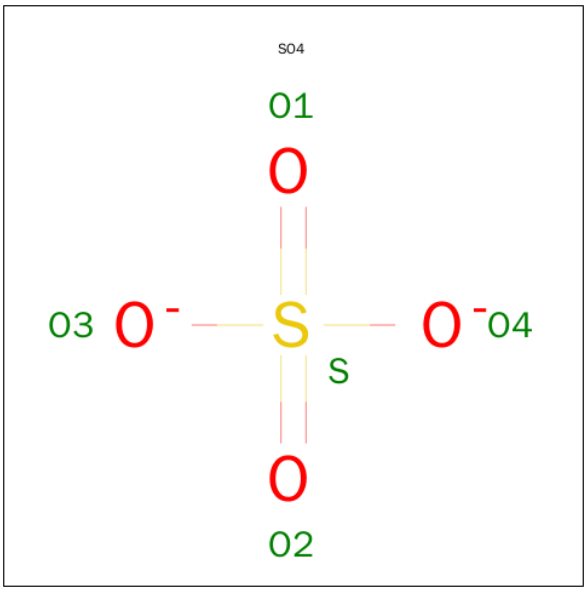
- Molecule 2 is a protein called ANTI-CITRULLINATED COLLAGEN TYPE II FAB ACC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1678	1053	282	337	6			
2	D	217	Total	C	N	O	S	0	0	0
			1678	1053	282	337	6			

- Molecule 3 is a protein called COLLAGEN DERIVED PEPTIDE PCII-CIT1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	0	0	0
			62	36	14	12			
3	F	7	Total	C	N	O	0	0	0
			53	31	12	10			

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



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

- Molecule 5 is water.

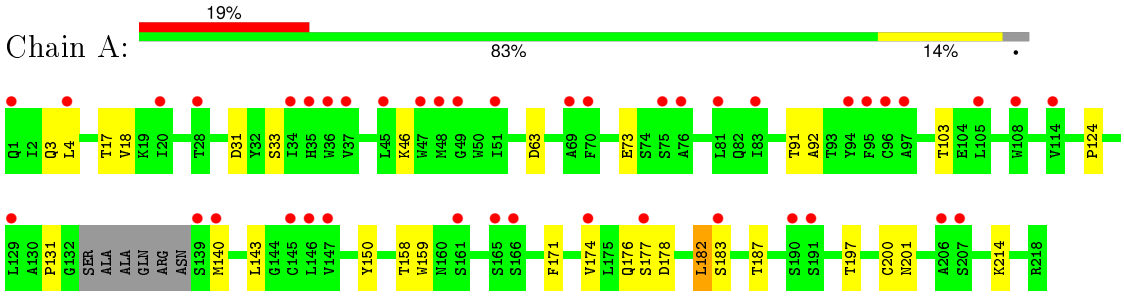
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	55	Total O 55 55	0	0
5	B	57	Total O 57 57	0	0
5	C	45	Total O 45 45	0	0
5	D	52	Total O 52 52	0	0
5	F	1	Total O 1 1	0	0

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.

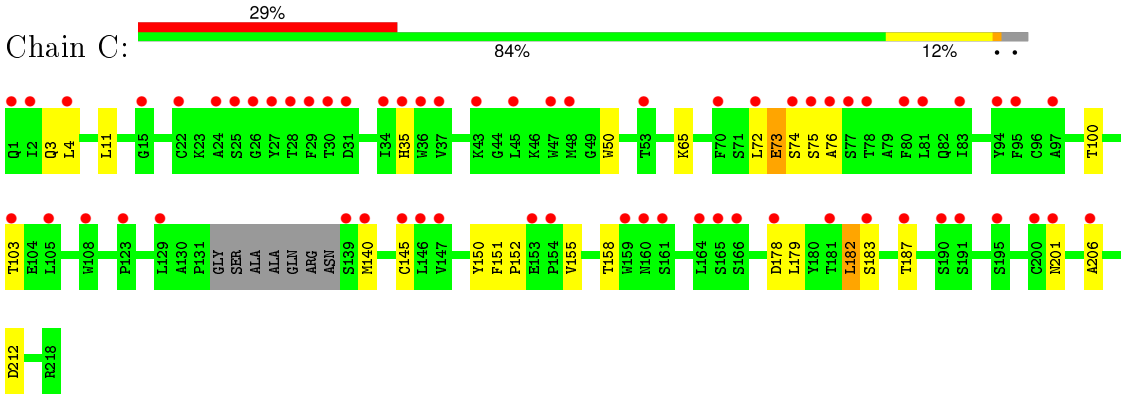
• Molecule 1: ANTI-CITRULLINATED COLLAGEN TYPE II FAB ACC4

Chain A:



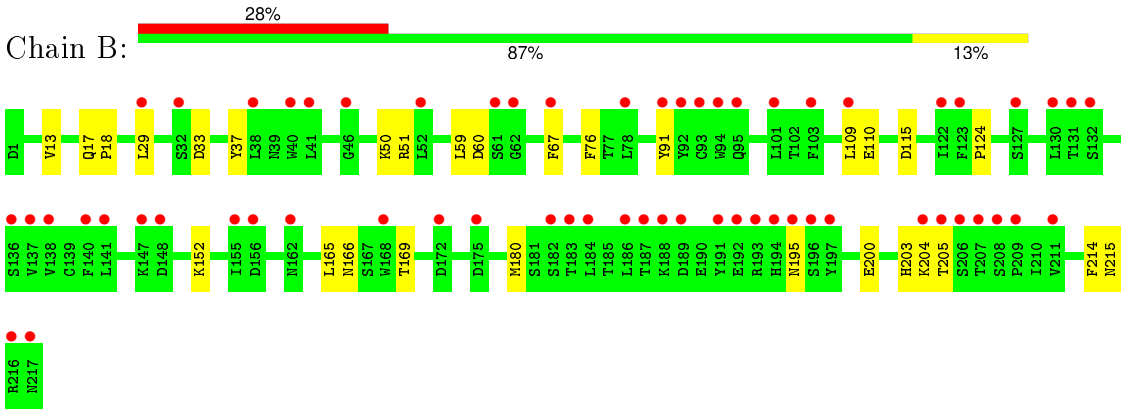
• Molecule 1: ANTI-CITRULLINATED COLLAGEN TYPE II FAB ACC4

Chain C:



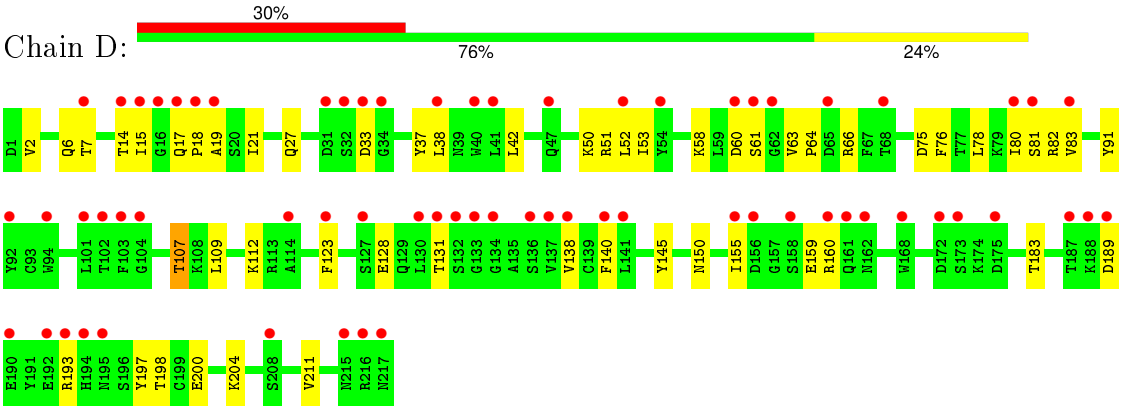
• Molecule 2: ANTI-CITRULLINATED COLLAGEN TYPE II FAB ACC4

Chain B:



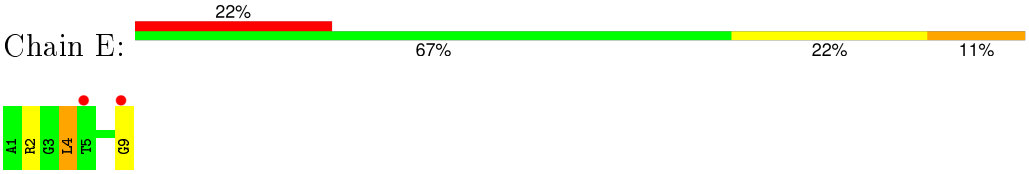
• Molecule 2: ANTI-CITRULLINATED COLLAGEN TYPE II FAB ACC4

Chain D:



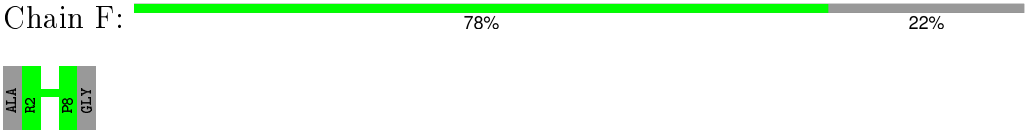
• Molecule 3: COLLAGEN DERIVED PEPTIDE PCII-CIT1

Chain E:



• Molecule 3: COLLAGEN DERIVED PEPTIDE PCII-CIT1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.20Å 127.80Å 71.90Å 90.00° 106.00° 90.00°	Depositor
Resolution (Å)	24.23 – 2.21 24.23 – 2.21	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.23-2.21) 97.2 (24.23-2.21)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.67 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.285 0.282 , 0.325	Depositor DCC
R_{free} test set	2407 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 48122 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6893	wwPDB-VP
Average B, all atoms (Å^2)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.72% 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: HYP, CIR, 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	0.72	0/1647	0.87	2/2254 (0.1%)
1	C	0.60	0/1643	0.92	4/2249 (0.2%)
2	B	0.60	0/1715	0.85	0/2330
2	D	0.66	0/1715	0.85	0/2330
3	E	0.82	0/40	1.38	1/48 (2.1%)
3	F	0.73	0/33	1.16	0/42
All	All	0.65	0/6793	0.88	7/9253 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	2	0
3	F	2	0
All	All	4	0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	75	SER	CB-CA-C	-14.40	82.73	110.10
1	C	73	GLU	CB-CA-C	-9.52	91.36	110.40
1	C	73	GLU	N-CA-C	6.02	127.26	111.00
1	A	33	SER	CB-CA-C	-5.98	98.73	110.10
1	C	74	SER	CB-CA-C	5.94	121.38	110.10
1	A	177	SER	N-CA-C	5.59	126.11	111.00
3	E	4	LEU	CA-CB-CG	5.20	127.27	115.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	2	CIR	C2
3	E	8	HYP	CG
3	F	2	CIR	C2
3	F	8	HYP	CG

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	1603	0	1572	27	0
1	C	1599	0	1569	27	0
2	B	1678	0	1639	22	0
2	D	1678	0	1639	48	0
3	E	62	0	62	3	0
3	F	53	0	54	0	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
5	A	55	0	0	1	0
5	B	57	0	0	0	0
5	C	45	0	0	2	0
5	D	52	0	0	5	0
5	F	1	0	0	0	0
All	All	6893	0	6535	118	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 9.

All (118) 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:C:100:THR:CG2	1:C:103:THR:HG23	1.90	1.00
1:C:100:THR:HG22	1:C:103:THR:HG23	1.49	0.95
1:A:158:THR:HG22	1:A:201:ASN:HB2	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:THR:CG2	1:C:103:THR:CG2	2.53	0.86
1:A:31:ASP:O	3:E:9:GLY:HA3	1.76	0.83
1:A:174:VAL:CG1	2:B:165:LEU:HD21	2.10	0.82
1:C:100:THR:HG21	1:C:103:THR:HG23	1.63	0.80
1:A:174:VAL:HG12	2:B:165:LEU:HD21	1.65	0.79
2:D:6:GLN:NE2	2:D:107:THR:HG22	1.97	0.79
1:C:100:THR:HG21	1:C:103:THR:CG2	2.13	0.79
2:D:21:ILE:HG21	2:D:107:THR:HG21	1.66	0.76
2:D:150:ASN:HB2	5:D:2041:HOH:O	1.85	0.76
1:C:158:THR:HG23	1:C:201:ASN:HB2	1.69	0.75
1:A:140:MET:CE	1:A:187:THR:HG22	2.17	0.75
1:A:140:MET:HE3	1:A:187:THR:HG22	1.67	0.74
1:C:201:ASN:HD22	1:C:212:ASP:CG	1.90	0.73
2:D:200:GLU:HG2	2:D:211:VAL:HG22	1.70	0.73
2:D:60:ASP:OD1	2:D:61:SER:N	2.22	0.72
2:D:38:LEU:HD22	2:D:76:PHE:CG	2.25	0.72
2:D:66:ARG:HD2	2:D:82:ARG:O	1.92	0.69
2:D:38:LEU:HD22	2:D:76:PHE:CD2	2.28	0.68
1:A:158:THR:CG2	1:A:201:ASN:HB2	2.23	0.68
1:C:158:THR:CG2	1:C:201:ASN:HB2	2.24	0.68
1:C:100:THR:HG22	1:C:103:THR:CG2	2.20	0.67
2:D:19:ALA:HB3	2:D:80:ILE:HB	1.78	0.65
1:C:183:SER:HB3	5:C:2036:HOH:O	1.95	0.65
1:A:3:GLN:C	1:A:4:LEU:HD12	2.16	0.65
2:D:91:TYR:CD1	2:D:109:LEU:HD13	2.32	0.65
1:A:197:THR:HG23	1:A:214:LYS:HE2	1.78	0.64
2:D:6:GLN:HE22	2:D:107:THR:HG22	1.63	0.61
2:B:51:ARG:HG2	2:B:60:ASP:OD2	2.00	0.61
2:D:33:ASP:OD2	2:D:37:TYR:OH	2.15	0.61
1:C:140:MET:CE	1:C:187:THR:HG22	2.31	0.61
1:A:182:LEU:HD23	1:A:183:SER:N	2.16	0.60
2:B:195:ASN:OD1	2:B:215:ASN:HB3	2.02	0.59
1:A:73:GLU:OE1	1:A:73:GLU:HA	2.03	0.58
2:D:42:LEU:HD13	2:D:91:TYR:CZ	2.38	0.58
2:D:63:VAL:HG13	2:D:64:PRO:HD2	1.86	0.57
1:C:100:THR:HG22	1:C:103:THR:O	2.05	0.57
1:A:174:VAL:HG11	2:B:165:LEU:HD21	1.85	0.57
1:C:100:THR:CG2	1:C:103:THR:HG22	2.35	0.56
2:B:59:LEU:HD21	2:B:67:PHE:O	2.05	0.56
2:B:124:PRO:HB3	2:B:214:PHE:CE2	2.40	0.56
1:A:182:LEU:HD23	1:A:182:LEU:C	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:LYS:HB3	2:B:200:GLU:HB2	1.87	0.56
1:C:178:ASP:O	1:C:179:LEU:HD13	2.04	0.56
2:D:21:ILE:CG2	2:D:107:THR:HG21	2.37	0.55
2:B:203:HIS:CE1	2:B:205:THR:HG23	2.43	0.54
2:D:21:ILE:HD13	2:D:107:THR:CG2	2.38	0.54
1:A:176:GLN:OE1	2:B:165:LEU:HD22	2.08	0.53
2:D:91:TYR:CE1	2:D:109:LEU:HD13	2.44	0.53
2:D:198:THR:CG2	2:D:211:VAL:HG13	2.39	0.53
1:C:11:LEU:HD11	1:C:151:PHE:HZ	1.74	0.53
2:D:21:ILE:HD13	2:D:107:THR:HG21	1.92	0.52
1:A:3:GLN:O	1:A:4:LEU:HD12	2.09	0.52
1:C:140:MET:HE2	1:C:187:THR:HG22	1.90	0.52
2:B:166:ASN:HB3	2:B:180:MET:HE3	1.93	0.51
2:D:189:ASP:O	2:D:193:ARG:HG3	2.10	0.51
1:A:46:LYS:NZ	1:A:63:ASP:OD2	2.29	0.51
2:D:18:PRO:HA	2:D:81:SER:O	2.11	0.50
1:C:201:ASN:ND2	1:C:212:ASP:CG	2.62	0.49
1:A:124:PRO:HB3	1:A:150:TYR:HB3	1.93	0.49
1:A:131:PRO:HD3	1:A:143:LEU:HD23	1.95	0.49
2:B:13:VAL:HG22	2:B:110:GLU:O	2.13	0.48
2:D:204:LYS:HB2	5:D:2037:HOH:O	2.13	0.48
1:C:182:LEU:HD23	1:C:183:SER:N	2.29	0.47
3:E:2:CIR:HN6	3:E:9:GLY:C	2.18	0.47
1:A:91:THR:O	1:A:92:ALA:HB2	2.15	0.47
1:A:73:GLU:HG2	5:A:2024:HOH:O	2.15	0.47
1:A:174:VAL:HG11	2:B:165:LEU:CD2	2.44	0.46
2:B:17:GLN:HB3	2:B:18:PRO:HD2	1.96	0.46
1:C:3:GLN:N	5:C:2002:HOH:O	2.49	0.46
2:D:66:ARG:CD	2:D:82:ARG:O	2.63	0.46
1:C:182:LEU:HD23	1:C:182:LEU:C	2.36	0.46
1:C:73:GLU:HG3	1:C:76:ALA:O	2.16	0.46
2:B:115:ASP:OD2	2:B:204:LYS:HE3	2.16	0.46
1:C:3:GLN:C	1:C:4:LEU:HD12	2.37	0.45
2:D:42:LEU:CB	2:D:52:LEU:HD11	2.47	0.45
2:D:83:VAL:HG12	2:D:83:VAL:O	2.16	0.45
2:D:21:ILE:HD11	2:D:109:LEU:HD11	1.97	0.45
1:C:35:HIS:ND1	1:C:50:TRP:HB3	2.31	0.45
2:D:7:THR:HG22	5:D:2005:HOH:O	2.17	0.45
2:D:14:THR:HG21	5:D:2009:HOH:O	2.17	0.45
1:A:197:THR:HG23	1:A:214:LYS:CE	2.47	0.44
1:A:159:TRP:CZ3	1:A:200:CYS:HB3	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:LYS:HB2	2:D:50:LYS:HE3	1.88	0.44
1:C:72:LEU:HG	1:C:73:GLU:H	1.82	0.44
2:D:128:GLU:OE1	2:D:128:GLU:N	2.51	0.44
2:D:52:LEU:HA	2:D:63:VAL:HG21	2.00	0.44
2:D:42:LEU:HB3	2:D:52:LEU:HD11	1.99	0.44
1:A:17:THR:HG22	1:A:18:VAL:N	2.32	0.43
2:D:138:VAL:HG22	2:D:183:THR:HG23	1.98	0.43
2:D:53:ILE:HD12	2:D:78:LEU:CD1	2.49	0.43
1:A:171:PHE:CD2	2:B:169:THR:HG23	2.53	0.43
2:D:51:ARG:NH2	2:D:60:ASP:OD1	2.52	0.43
2:D:60:ASP:HB3	2:D:63:VAL:CG2	2.48	0.43
2:D:63:VAL:CG1	2:D:64:PRO:HD2	2.48	0.43
1:C:152:PRO:HD2	1:C:206:ALA:CB	2.48	0.43
2:D:2:VAL:HG22	2:D:27:GLN:CG	2.49	0.43
2:D:200:GLU:CG	2:D:211:VAL:HG22	2.45	0.43
2:D:123:PHE:HE1	2:D:140:PHE:HD2	1.67	0.43
2:D:58:LYS:NZ	5:D:2018:HOH:O	2.51	0.42
2:D:112:LYS:HA	2:D:145:TYR:OH	2.19	0.42
1:C:150:TYR:CE1	1:C:155:VAL:HG13	2.54	0.42
2:B:29:LEU:HD12	2:B:76:PHE:CE1	2.54	0.42
2:D:155:ILE:HD12	2:D:197:TYR:CD2	2.53	0.42
2:B:50:LYS:HB2	2:B:50:LYS:HE3	1.83	0.42
2:B:91:TYR:HE1	2:B:109:LEU:HD22	1.85	0.41
2:B:33:ASP:OD2	2:B:37:TYR:OH	2.32	0.41
1:A:174:VAL:CG1	2:B:165:LEU:CD2	2.88	0.41
1:A:140:MET:HE2	1:A:187:THR:HG22	1.96	0.41
2:D:60:ASP:HB3	2:D:63:VAL:HG21	2.01	0.41
1:C:65:LYS:HE2	3:E:4:LEU:HD22	2.03	0.41
2:D:17:GLN:HB3	2:D:18:PRO:HD2	2.02	0.41
2:D:131:THR:HG22	2:D:131:THR:O	2.21	0.41
2:D:159:GLU:HG2	2:D:160:ARG:H	1.86	0.40
2:B:195:ASN:O	2:B:215:ASN:HA	2.22	0.40
2:D:14:THR:O	2:D:15:ILE:C	2.58	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	208/218 (95%)	198 (95%)	10 (5%)	0	100	100
1	C	207/218 (95%)	188 (91%)	19 (9%)	0	100	100
2	B	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
2	D	215/217 (99%)	201 (94%)	14 (6%)	0	100	100
3	E	4/9 (44%)	4 (100%)	0	0	100	100
3	F	4/9 (44%)	4 (100%)	0	0	100	100
All	All	853/888 (96%)	804 (94%)	49 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	180/185 (97%)	177 (98%)	3 (2%)	68	80
1	C	180/185 (97%)	178 (99%)	2 (1%)	80	89
2	B	193/194 (100%)	193 (100%)	0	100	100
2	D	193/194 (100%)	191 (99%)	2 (1%)	82	90
3	E	3/3 (100%)	3 (100%)	0	100	100
3	F	3/3 (100%)	3 (100%)	0	100	100
All	All	752/764 (98%)	745 (99%)	7 (1%)	84	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	THR
1	A	178	ASP
1	A	182	LEU
1	C	145	CYS
1	C	182	LEU
2	D	75	ASP
2	D	107	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	194	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)

4 non-standard protein/DNA/RNA residues 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	CIR	E	2	3	9,10,11	0.89	1 (11%)	9,11,13	3.59	4 (44%)
3	HYP	E	8	3	7,8,9	0.80	0	5,10,12	2.17	2 (40%)
3	CIR	F	2	3	9,10,11	0.67	0	9,11,13	3.22	5 (55%)
3	HYP	F	8	3	7,8,9	0.82	0	5,10,12	0.98	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	CIR	E	2	3	1/1/2/4	0/7/9/11	0/0/0/0
3	HYP	E	8	3	1/1/2/4	0/0/11/13	0/1/1/1
3	CIR	F	2	3	1/1/2/4	0/7/9/11	0/0/0/0
3	HYP	F	8	3	1/1/2/4	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	CIR	C3-C2	-2.46	1.51	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2	CIR	O7-C7-N6	-3.23	118.92	122.04
3	E	2	CIR	O1-C1-C2	-2.73	118.38	125.49
3	E	8	HYP	OD1-CG-CD	-2.58	104.87	110.47
3	E	2	CIR	O7-C7-N8	-2.50	119.02	123.30
3	F	2	CIR	O1-C1-C2	-2.08	120.06	125.49
3	F	2	CIR	O7-C7-N8	-2.04	119.80	123.30
3	E	2	CIR	O7-C7-N6	2.52	124.47	122.04
3	E	8	HYP	CB-CG-CD	3.29	107.21	103.14
3	F	2	CIR	N8-C7-N6	4.18	121.28	116.17
3	F	2	CIR	C3-C2-N2	7.40	131.54	110.52
3	E	2	CIR	C3-C2-N2	9.53	137.61	110.52

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	8	HYP	CG
3	E	8	HYP	CG
3	F	2	CIR	C2
3	E	2	CIR	C2

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	CIR	1	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	$\#\|Z\| > 2$
4	SO4	A	1219	-	4,4,4	0.43	0	6,6,6	0.67	0
4	SO4	C	1219	-	4,4,4	0.21	0	6,6,6	0.45	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
4	SO4	A	1219	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1219	-	-	0/0/0/0	0/0/0/0

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

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	212/218 (97%)	1.09	42 (19%) 1 1	2, 7, 12, 16	0
1	C	211/218 (96%)	1.57	63 (29%) 1 0	2, 9, 15, 20	0
2	B	217/217 (100%)	1.50	61 (28%) 1 1	2, 17, 40, 43	0
2	D	217/217 (100%)	1.61	66 (30%) 1 0	2, 7, 16, 21	0
3	E	7/9 (77%)	1.43	2 (28%) 1 0	2, 2, 6, 12	0
3	F	5/9 (55%)	0.73	0 100 100	5, 6, 10, 16	0
All	All	869/888 (97%)	1.44	234 (26%) 1 1	2, 8, 31, 43	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	131	THR	9.0
2	B	138	VAL	6.9
1	C	76	ALA	6.5
2	D	158	SER	6.5
1	C	77	SER	6.0
2	B	137	VAL	6.0
1	C	105	LEU	5.8
2	D	132	SER	5.8
2	D	18	PRO	5.6
1	C	75	SER	5.5
1	A	36	TRP	5.5
1	C	74	SER	5.4
2	D	215	ASN	5.4
2	B	196	SER	5.2
1	C	26	GLY	5.1
2	B	131	THR	5.1
1	A	105	LEU	5.1
2	B	207	THR	5.0
2	B	189	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	162	ASN	4.9
1	A	34	ILE	4.8
1	C	146	LEU	4.8
2	D	32	SER	4.7
1	C	37	VAL	4.7
2	D	217	ASN	4.7
2	D	189	ASP	4.7
2	D	138	VAL	4.6
1	C	36	TRP	4.5
2	D	193	ARG	4.5
1	C	28	THR	4.5
1	A	146	LEU	4.4
2	D	60	ASP	4.4
1	A	81	LEU	4.4
2	B	38	LEU	4.4
2	B	187	THR	4.3
1	A	97	ALA	4.3
2	D	33	ASP	4.3
1	C	129	LEU	4.2
1	C	165	SER	4.2
1	C	27	TYR	4.2
2	D	40	TRP	4.2
2	B	41	LEU	4.2
1	A	75	SER	4.1
2	D	134	GLY	4.1
2	B	194	HIS	4.1
1	C	34	ILE	4.1
1	A	45	LEU	4.1
1	C	1	GLN	4.1
2	D	61	SER	4.0
2	D	94	TRP	4.0
1	A	140	MET	4.0
2	B	140	PHE	4.0
1	A	37	VAL	3.9
1	A	20	ILE	3.9
1	C	25	SER	3.9
1	A	190	SER	3.9
2	B	132	SER	3.8
2	D	187	THR	3.8
2	D	188	LYS	3.8
2	B	206	SER	3.8
1	C	81	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	184	LEU	3.8
2	D	130	LEU	3.8
2	B	94	TRP	3.7
2	B	32	SER	3.7
1	C	161	SER	3.7
1	A	94	TYR	3.7
2	D	195	ASN	3.7
2	D	41	LEU	3.7
1	C	2	ILE	3.7
2	B	40	TRP	3.6
1	C	139	SER	3.6
1	C	195	SER	3.6
2	D	38	LEU	3.6
2	B	205	THR	3.5
1	C	166	SER	3.5
2	D	127	SER	3.5
2	B	217	ASN	3.5
2	D	123	PHE	3.5
1	A	139	SER	3.5
1	A	95	PHE	3.5
2	B	155	ILE	3.5
2	B	195	ASN	3.4
2	D	19	ALA	3.4
2	B	188	LYS	3.4
1	C	78	THR	3.4
2	B	52	LEU	3.4
1	C	24	ALA	3.4
2	B	193	ARG	3.3
2	D	47	GLN	3.3
2	D	7	THR	3.3
2	D	216	ARG	3.3
2	B	211	VAL	3.3
1	C	201	ASN	3.2
1	A	177	SER	3.2
2	B	91	TYR	3.2
2	D	34	GLY	3.2
1	C	147	VAL	3.2
1	A	48	MET	3.2
2	B	123	PHE	3.1
2	B	208	SER	3.1
2	B	216	ARG	3.1
2	B	156	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	187	THR	3.1
2	D	103	PHE	3.0
2	D	162	ASN	3.0
2	B	130	LEU	3.0
2	B	103	PHE	3.0
1	C	145	CYS	3.0
2	D	62	GLY	3.0
2	B	182	SER	3.0
2	D	173	SER	3.0
2	D	175	ASP	2.9
2	D	137	VAL	2.9
2	D	101	LEU	2.9
2	D	194	HIS	2.9
2	D	65	ASP	2.9
1	C	22	CYS	2.9
1	C	15	GLY	2.9
2	B	122	ILE	2.9
2	D	15	ILE	2.9
2	B	101	LEU	2.9
2	D	156	ASP	2.9
2	D	83	VAL	2.9
2	D	80	ILE	2.9
2	D	81	SER	2.9
2	D	133	GLY	2.8
1	A	206	ALA	2.8
1	C	30	THR	2.8
2	B	204	LYS	2.8
1	A	166	SER	2.8
1	A	108	TRP	2.8
1	C	123	PRO	2.8
1	C	183	SER	2.8
1	C	72	LEU	2.8
1	C	47	TRP	2.8
1	C	154	PRO	2.8
1	C	95	PHE	2.7
1	C	190	SER	2.7
2	B	172	ASP	2.7
2	B	46	GLY	2.7
1	A	83	ILE	2.7
2	D	155	ILE	2.7
1	C	35	HIS	2.7
2	D	68	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	209	PRO	2.7
1	C	48	MET	2.7
1	A	1	GLN	2.6
2	B	67	PHE	2.6
1	C	94	TYR	2.6
1	C	97	ALA	2.6
1	C	31	ASP	2.6
1	A	147	VAL	2.5
1	C	70	PHE	2.5
2	B	62	GLY	2.5
2	B	168	TRP	2.5
1	A	49	GLY	2.5
2	D	31	ASP	2.5
2	D	168	TRP	2.5
2	B	192	GLU	2.5
2	B	148	ASP	2.5
2	B	136	SER	2.4
2	D	14	THR	2.4
2	B	186	LEU	2.4
2	D	54	TYR	2.4
1	C	191	SER	2.4
2	D	161	GLN	2.4
1	A	207	SER	2.4
1	C	140	MET	2.4
2	B	109	LEU	2.4
1	C	178	ASP	2.4
1	A	76	ALA	2.4
3	E	5	THR	2.4
1	C	153	GLU	2.4
1	C	164	LEU	2.4
2	D	141	LEU	2.4
2	D	16	GLY	2.4
1	C	159	TRP	2.4
1	A	4	LEU	2.4
2	B	29	LEU	2.4
2	D	52	LEU	2.4
1	C	4	LEU	2.3
1	C	45	LEU	2.3
2	B	92	TYR	2.3
2	D	104	GLY	2.3
1	C	83	ILE	2.3
2	D	102	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	161	SER	2.3
2	D	17	GLN	2.3
2	B	183	THR	2.3
1	A	129	LEU	2.3
1	A	96	CYS	2.3
2	D	114	ALA	2.3
2	D	160	ARG	2.3
2	D	92	TYR	2.3
1	C	29	PHE	2.3
1	C	43	LYS	2.3
1	A	174	VAL	2.2
1	C	160	ASN	2.2
1	A	191	SER	2.2
1	C	200	CYS	2.2
2	D	172	ASP	2.2
1	A	114	VAL	2.2
2	D	140	PHE	2.2
1	A	183	SER	2.2
1	A	47	TRP	2.2
1	C	108	TRP	2.2
2	B	191	TYR	2.2
2	B	93	CYS	2.2
2	D	136	SER	2.2
1	A	28	THR	2.2
1	A	69	ALA	2.1
1	A	145	CYS	2.1
2	B	61	SER	2.1
2	B	78	LEU	2.1
1	C	206	ALA	2.1
1	A	165	SER	2.1
2	D	192	GLU	2.1
2	B	175	ASP	2.1
3	E	9	GLY	2.1
1	A	51	ILE	2.1
1	A	70	PHE	2.1
1	C	181	THR	2.1
2	D	190	GLU	2.1
2	D	208	SER	2.1
1	C	53	THR	2.0
1	C	103	THR	2.0
2	B	197	TYR	2.0
2	B	127	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	80	PHE	2.0
2	B	95	GLN	2.0
2	B	141	LEU	2.0
2	B	147	LYS	2.0
1	A	35	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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	HYP	F	8	8/9	0.84	0.17	-	15,15,16,19	0
3	HYP	E	8	8/9	0.84	0.15	-	8,9,10,17	0
3	CIR	F	2	11/12	0.82	0.17	-	11,14,23,24	0
3	CIR	E	2	11/12	0.87	0.22	-	2,3,6,7	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	A	1219	5/5	0.95	0.12	-1.70	13,16,18,19	0
4	SO4	C	1219	5/5	0.91	0.15	-3.44	33,33,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.