



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2022 – 06:03 PM EST

PDB ID : 7SG2
Title : XPA5 TCR in complex with HLA-DQ2-omega1
Authors : Ciacchi, L.; Farenc, C.; Petersen, J.; Reid, H.H.; Rossjohn, J.
Deposited on : 2021-10-04
Resolution : 3.10 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
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)	:	2.26

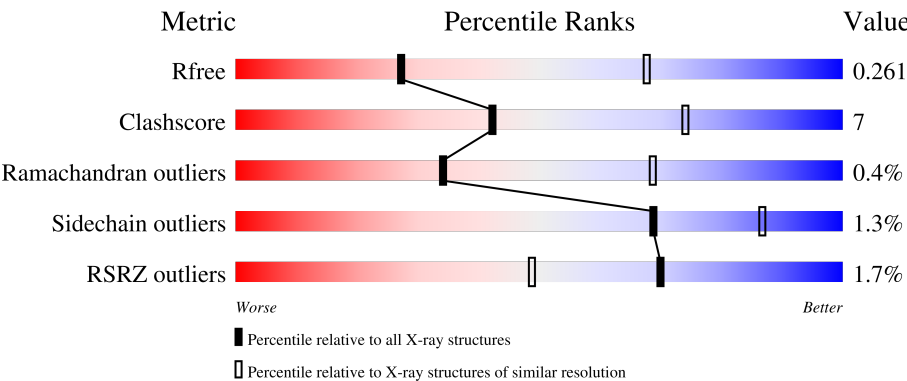
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 $\leq 5\%$. 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	183	<div> <div>3%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	F	183	<div> <div>83%</div> <div>14%</div> <div>..</div> </div>
2	B	205	<div> <div>3%</div> <div>62%</div> <div>23%</div> <div>15%</div> </div>
2	G	205	<div> <div>66%</div> <div>21%</div> <div>12%</div> </div>
3	D	203	<div> <div>5%</div> <div>79%</div> <div>13%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	203	<div><div></div><div>75%</div><div>9%</div><div>16%</div></div>
4	E	246	<div><div></div><div>84%</div><div>14%</div><div></div></div>
4	J	246	<div><div></div><div>%</div><div>80%</div><div>13%</div><div>6%</div></div>
5	C	13	<div><div></div><div>54%</div><div>46%</div></div>
5	H	13	<div><div></div><div>69%</div><div>31%</div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12551 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 II histocompatibility antigen, DQ alpha 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1422	917	233	269	3			
1	F	178	Total	C	N	O	S	0	0	0
			1421	915	233	270	3			

- Molecule 2 is a protein called MHC class II HLA-DQ-beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1441	912	255	267	7			
2	G	180	Total	C	N	O	S	0	0	0
			1479	934	264	274	7			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	GLY	-	expression tag	UNP O19712
B	-11	GLY	-	expression tag	UNP O19712
B	-10	SER	-	expression tag	UNP O19712
B	-9	ILE	-	expression tag	UNP O19712
B	-8	GLU	-	expression tag	UNP O19712
B	-7	GLY	-	expression tag	UNP O19712
B	-6	ARG	-	expression tag	UNP O19712
B	-5	GLY	-	expression tag	UNP O19712
B	-4	GLY	-	expression tag	UNP O19712
B	-3	SER	-	expression tag	UNP O19712
B	-2	GLY	-	expression tag	UNP O19712
B	-1	ALA	-	expression tag	UNP O19712
B	0	SER	-	expression tag	UNP O19712
G	-12	GLY	-	expression tag	UNP O19712
G	-11	GLY	-	expression tag	UNP O19712
G	-10	SER	-	expression tag	UNP O19712

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-9	ILE	-	expression tag	UNP O19712
G	-8	GLU	-	expression tag	UNP O19712
G	-7	GLY	-	expression tag	UNP O19712
G	-6	ARG	-	expression tag	UNP O19712
G	-5	GLY	-	expression tag	UNP O19712
G	-4	GLY	-	expression tag	UNP O19712
G	-3	SER	-	expression tag	UNP O19712
G	-2	GLY	-	expression tag	UNP O19712
G	-1	ALA	-	expression tag	UNP O19712
G	0	SER	-	expression tag	UNP O19712

- Molecule 3 is a protein called T-cell receptor, xpa5, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	188	Total	C	N	O	S	0	0	0
			1478	930	248	291	9			
3	I	170	Total	C	N	O	S	0	0	0
			1322	823	223	267	9			

- Molecule 4 is a protein called T-cell receptor, xpa5, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	242	Total	C	N	O	S	0	0	0
			1903	1198	325	371	9			
4	J	232	Total	C	N	O	S	0	0	0
			1822	1150	313	350	9			

- Molecule 5 is a protein called DQ2-glia-omega1 peptide.

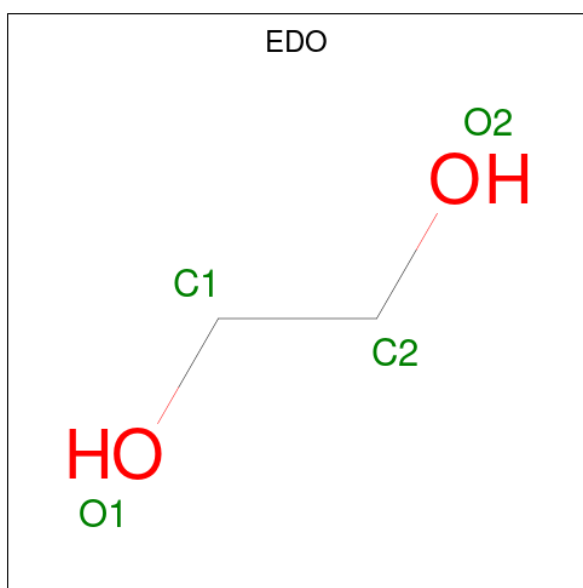
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	13	Total	C	N	O	0	0	0
			103	68	16	19			
5	H	13	Total	C	N	O	0	0	0
			103	68	16	19			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



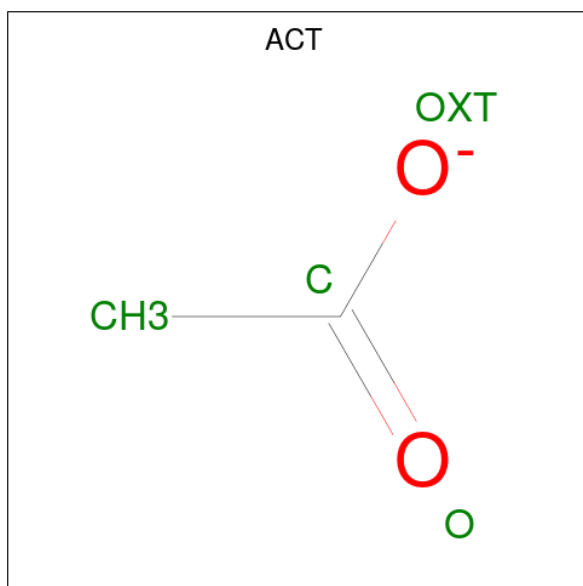
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	J	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Ca	0	0
			1	1		
9	E	1	Total	Ca	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	2	Total	O	0	0
			2	2		
10	B	3	Total	O	0	0
			3	3		

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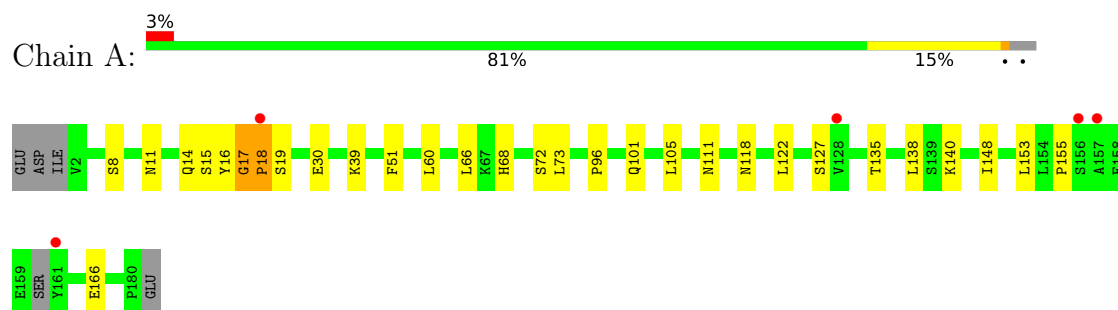
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	F	1	Total 1	O 1	0	0
10	E	1	Total 1	O 1	0	0

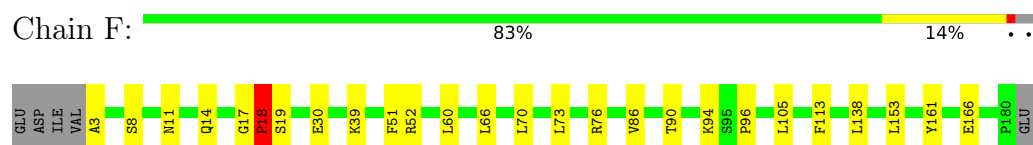
3 Residue-property plots [i](#)

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.

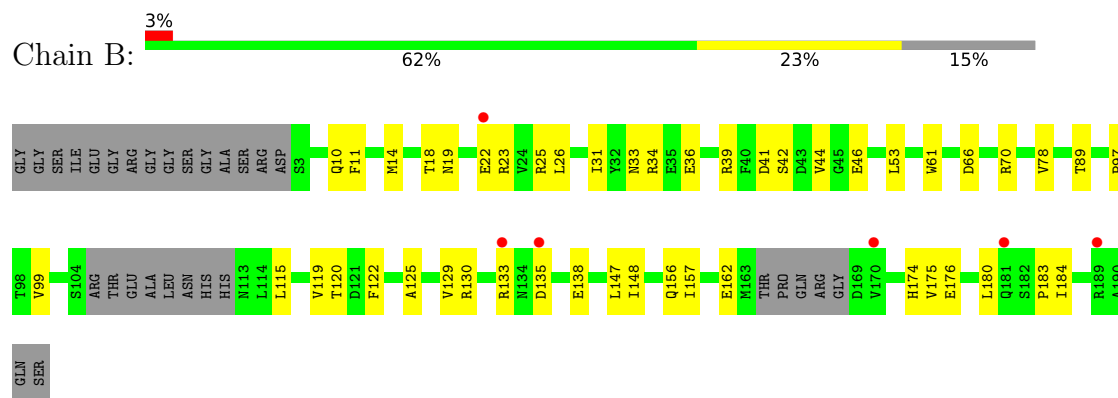
- Molecule 1: HLA class II histocompatibility antigen, DQ alpha 1 chain



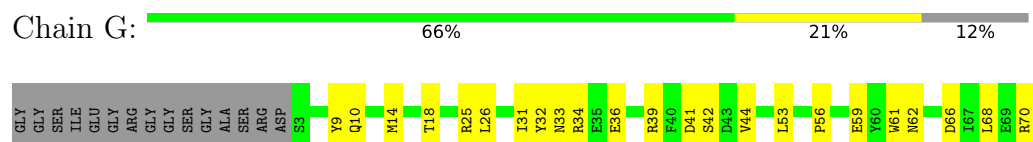
- Molecule 1: HLA class II histocompatibility antigen, DQ alpha 1 chain



- Molecule 2: MHC class II HLA-DQ-beta-1

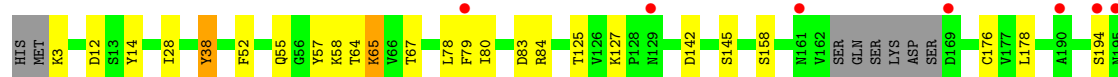
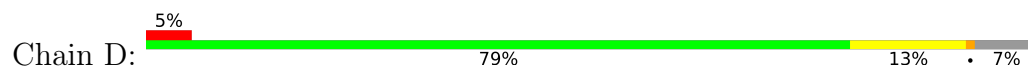


- Molecule 2: MHC class II HLA-DQ-beta-1

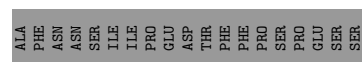
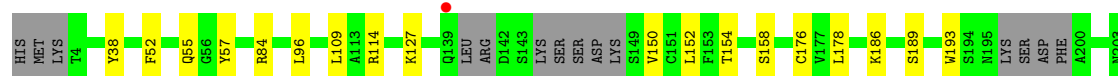




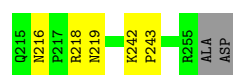
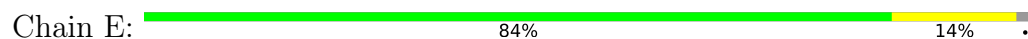
- Molecule 3: T-cell receptor, xpa5, alpha chain



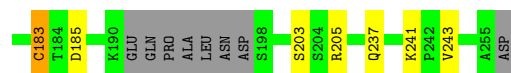
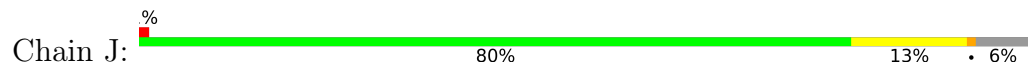
- Molecule 3: T-cell receptor, xpa5, alpha chain



- Molecule 4: T-cell receptor, xpa5, beta chain



- Molecule 4: T-cell receptor, xpa5, beta chain

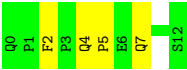


- Molecule 5: DQ2-glia-omega1 peptide





- Molecule 5: DQ2-glia-omega1 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.25Å 75.11Å 216.43Å 90.00° 103.16° 90.00°	Depositor
Resolution (Å)	45.44 – 3.10 45.44 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.44-3.10) 99.9 (45.44-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.218 , 0.259 0.222 , 0.261	Depositor DCC
R_{free} test set	1956 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.027 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12551	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CA, NAG, ACT, EDO

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	0.32	0/1463	0.52	0/1997
1	F	0.31	0/1463	0.50	0/1998
2	B	0.26	0/1472	0.49	0/1998
2	G	0.29	0/1512	0.48	0/2054
3	D	0.35	0/1509	0.56	0/2048
3	I	0.24	0/1346	0.44	0/1827
4	E	0.29	0/1950	0.49	0/2656
4	J	0.30	0/1866	0.51	0/2538
5	C	0.41	0/109	0.56	0/150
5	H	0.31	0/109	0.37	0/150
All	All	0.30	0/12799	0.50	0/17416

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1422	0	1371	23	0
1	F	1421	0	1368	22	0
2	B	1441	0	1407	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1479	0	1447	37	0
3	D	1478	0	1423	19	0
3	I	1322	0	1261	17	0
4	E	1903	0	1824	20	0
4	J	1822	0	1750	21	0
5	C	103	0	93	6	0
5	H	103	0	93	6	0
6	A	14	0	13	0	0
6	F	14	0	13	1	0
7	A	4	0	6	0	0
7	J	8	0	12	0	0
8	A	4	0	3	1	0
8	F	4	0	3	0	0
9	B	1	0	0	0	0
9	E	1	0	0	0	0
10	A	2	0	0	0	0
10	B	3	0	0	0	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
All	All	12551	0	12087	169	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 (169) 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:F:11:ASN:HB3	1:F:66:LEU:HD11	1.62	0.82
1:A:11:ASN:HB3	1:A:66:LEU:HD11	1.62	0.80
3:I:109:LEU:HD12	3:I:114:ARG:HH12	1.50	0.76
3:I:109:LEU:CD1	3:I:114:ARG:HH12	1.98	0.76
3:I:109:LEU:HD12	3:I:114:ARG:NH1	2.03	0.74
1:F:76:ARG:HH12	2:G:56:PRO:HG2	1.52	0.73
1:A:96:PRO:HD3	2:B:120:THR:HG21	1.70	0.73
3:D:58:LYS:HA	3:D:84:ARG:HD3	1.71	0.70
3:D:65:LYS:HB2	3:D:79:PHE:HA	1.76	0.68
4:J:77:PRO:HG2	4:J:90:THR:HB	1.75	0.68
1:F:96:PRO:HD3	2:G:120:THR:HG21	1.77	0.67
4:E:38:MET:HB2	4:E:107:ALA:HB3	1.78	0.66
4:E:77:PRO:HG2	4:E:90:THR:HB	1.77	0.66
3:I:57:TYR:O	3:I:84:ARG:NH1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:LEU:HB3	2:B:42:SER:HB3	1.79	0.65
3:I:176:CYS:SG	4:J:205:ARG:NH1	2.70	0.65
2:G:125:ALA:HB1	2:G:147:LEU:HD21	1.79	0.64
4:J:67:TYR:CE1	4:J:73:ILE:HG12	2.33	0.64
1:A:135:THR:HG22	1:A:148:ILE:H	1.64	0.63
4:E:4:ILE:HD11	4:E:106:VAL:HB	1.78	0.63
2:G:62:ASN:HA	2:G:68:LEU:HD21	1.81	0.63
2:G:26:LEU:HB3	2:G:42:SER:HB3	1.80	0.63
2:B:125:ALA:HB1	2:B:147:LEU:HD21	1.80	0.62
2:B:10:GLN:HB2	2:B:31:ILE:HB	1.82	0.61
1:A:68:HIS:HE1	5:C:9:PHE:O	1.82	0.61
4:J:43:ARG:HB2	4:J:53:ILE:HD11	1.83	0.61
2:B:133:ARG:NH2	2:B:162:GLU:O	2.33	0.60
2:B:133:ARG:HG3	2:B:138:GLU:HG3	1.84	0.59
3:I:154:THR:HG22	3:I:189:SER:HB3	1.83	0.59
3:D:28:ILE:HG21	3:D:84:ARG:O	2.03	0.58
1:A:39:LYS:HG2	1:A:60:LEU:HD11	1.84	0.58
4:J:26:ASP:OD1	4:J:27:SER:N	2.37	0.58
4:J:38:MET:HB2	4:J:107:ALA:HB3	1.84	0.58
2:B:31:ILE:HG22	2:B:33:ASN:O	2.03	0.57
1:F:39:LYS:HG2	1:F:60:LEU:HD11	1.86	0.57
2:B:41:ASP:HB3	2:B:44:VAL:HG22	1.87	0.57
2:G:99:VAL:HG12	2:G:119:VAL:HG22	1.86	0.56
3:D:58:LYS:CA	3:D:84:ARG:HD3	2.36	0.56
2:B:70:ARG:NH1	3:D:55:GLN:OE1	2.34	0.56
1:F:17:GLY:O	1:F:18:PRO:C	2.43	0.56
2:B:18:THR:HB	2:B:23:ARG:HB2	1.86	0.56
2:G:66:ASP:OD2	4:J:113:THR:OG1	2.23	0.56
2:B:133:ARG:HG3	2:B:138:GLU:CG	2.36	0.56
3:D:178:LEU:HB3	4:E:184:CYS:HB2	1.87	0.56
3:D:176:CYS:SG	4:E:206:ARG:NH1	2.78	0.55
2:G:25:ARG:NH2	2:G:41:ASP:OD2	2.40	0.55
2:B:25:ARG:NH2	2:B:41:ASP:OD2	2.37	0.55
4:J:131:LYS:HD2	4:J:237:GLN:NE2	2.21	0.55
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.89	0.54
4:E:164:PHE:HB3	4:E:165:PRO:HD3	1.89	0.54
2:G:181:GLN:H	2:G:181:GLN:CD	2.11	0.54
3:D:65:LYS:HD2	3:D:78:LEU:O	2.07	0.54
3:D:52:PHE:HZ	3:D:55:GLN:HB2	1.73	0.54
1:A:17:GLY:O	1:A:18:PRO:C	2.47	0.53
4:E:7:LYS:HB3	4:E:8:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:ASP:OD2	4:E:113:THR:OG1	2.26	0.53
4:J:15:ARG:NE	4:J:128:GLU:OE1	2.40	0.53
3:D:58:LYS:HG2	3:D:58:LYS:O	2.09	0.53
2:G:32:TYR:CE1	2:G:33:ASN:ND2	2.77	0.53
4:E:216:ASN:OD1	4:E:218:ARG:HG2	2.09	0.53
3:I:150:VAL:HG22	3:I:193:TRP:HB3	1.92	0.52
2:B:135:ASP:OD1	2:B:135:ASP:O	2.28	0.52
1:F:30:GLU:HB2	1:F:138:LEU:HD21	1.91	0.52
3:D:64:THR:H	3:D:80:ILE:HD12	1.75	0.52
2:G:70:ARG:NH1	3:I:55:GLN:HE21	2.08	0.52
4:J:8:PRO:HD2	4:J:21:ILE:HG23	1.92	0.52
1:A:17:GLY:O	1:A:19:SER:N	2.42	0.52
4:J:25:VAL:HG21	4:J:106:VAL:HG21	1.92	0.52
4:J:185:ASP:OD2	4:J:203:SER:OG	2.28	0.51
2:B:99:VAL:HG12	2:B:119:VAL:HG22	1.92	0.51
3:I:52:PHE:HZ	3:I:55:GLN:HB2	1.76	0.51
2:G:41:ASP:HB3	2:G:44:VAL:HG22	1.93	0.51
4:J:4:ILE:HD11	4:J:106:VAL:HB	1.92	0.51
3:D:194:SER:HB3	3:D:199:PHE:CG	2.46	0.51
4:E:43:ARG:HB2	4:E:53:ILE:HD11	1.92	0.51
1:A:101:GLN:O	1:A:155:PRO:HD2	2.12	0.50
2:G:180:LEU:HD13	2:G:184:ILE:HG13	1.93	0.50
3:D:52:PHE:CZ	3:D:55:GLN:HB2	2.47	0.50
2:G:99:VAL:HG11	2:G:175:VAL:HG21	1.94	0.49
2:B:129:VAL:HG22	2:B:175:VAL:HG22	1.94	0.49
2:B:130:ARG:HB2	2:B:174:HIS:HB3	1.94	0.49
1:A:30:GLU:HB2	1:A:138:LEU:HD21	1.93	0.49
4:J:94:MET:HE2	4:J:124:LEU:HD21	1.93	0.49
1:F:105:LEU:HG	1:F:153:LEU:HD21	1.93	0.49
8:A:203:ACT:H2	2:B:34:ARG:HH22	1.77	0.48
1:F:166:GLU:O	6:F:201:NAG:H83	2.13	0.48
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.95	0.48
1:F:70:LEU:HD13	2:G:9:TYR:HB2	1.95	0.48
3:I:152:LEU:HG	3:I:154:THR:HG23	1.96	0.48
3:I:52:PHE:CZ	3:I:55:GLN:HB2	2.49	0.47
3:I:109:LEU:CD1	3:I:114:ARG:NH1	2.67	0.47
2:B:180:LEU:HD13	2:B:184:ILE:HG13	1.95	0.47
1:F:14:GLN:HG2	1:F:19:SER:HB2	1.96	0.47
2:G:36:GLU:OE2	2:G:39:ARG:HB3	2.14	0.47
2:G:78:VAL:HG22	5:H:2:PHE:HD2	1.78	0.47
3:I:178:LEU:HB3	4:J:183:CYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HG	1:A:153:LEU:HD21	1.97	0.47
4:E:25:VAL:HG21	4:E:106:VAL:HG21	1.97	0.47
2:B:61:TRP:CE2	5:C:7:GLN:HB2	2.49	0.47
3:D:12:ASP:OD1	3:D:125:THR:OG1	2.32	0.47
3:I:109:LEU:HD13	3:I:114:ARG:HH12	1.77	0.47
2:B:36:GLU:OE2	2:B:39:ARG:HB3	2.15	0.47
1:A:51:PHE:HE2	2:B:89:THR:HG21	1.80	0.46
3:D:142:ASP:HB3	3:D:145:SER:O	2.15	0.46
1:F:3:ALA:N	2:G:18:THR:HG1	2.13	0.46
1:F:51:PHE:HE2	2:G:89:THR:HG21	1.79	0.46
1:A:68:HIS:CE1	5:C:9:PHE:O	2.67	0.46
3:I:96:LEU:HD11	3:I:186:LYS:HD3	1.98	0.46
3:D:127:LYS:HB3	3:D:158:SER:HB3	1.97	0.46
4:E:95:SER:OG	4:E:97:GLU:OE1	2.33	0.46
4:J:12:ILE:HD11	4:J:164:PRO:HG3	1.98	0.46
1:A:11:ASN:HB2	2:B:11:PHE:HB3	1.99	0.45
4:E:143:PRO:HD2	4:E:214:TRP:CZ2	2.52	0.45
2:G:119:VAL:HB	2:G:157:ILE:HG22	1.98	0.45
4:J:12:ILE:CD1	4:J:164:PRO:HG3	2.47	0.45
4:J:143:PRO:O	4:J:144:SER:HB3	2.17	0.45
2:G:61:TRP:CE2	5:H:7:GLN:HB2	2.52	0.45
2:G:70:ARG:HH11	3:I:55:GLN:HE21	1.63	0.45
4:E:95:SER:OG	4:E:96:PRO:HD2	2.17	0.45
2:G:26:LEU:HD11	5:H:4:GLN:NE2	2.33	0.44
2:G:122:PHE:CZ	2:G:127:ILE:HD13	2.52	0.44
2:B:119:VAL:HB	2:B:157:ILE:HG22	1.99	0.44
1:F:14:GLN:HE21	1:F:19:SER:HB2	1.82	0.44
2:G:152:ASP:OD1	2:G:154:THR:OG1	2.34	0.44
4:J:241:LYS:HE3	4:J:243:VAL:HG22	1.99	0.44
4:E:72:VAL:HG12	4:E:74:ASP:H	1.81	0.44
2:B:148:ILE:HB	2:B:156:GLN:HG3	1.99	0.44
2:B:176:GLU:HG2	2:B:183:PRO:HB3	1.99	0.44
1:F:14:GLN:CG	1:F:19:SER:HB2	2.48	0.44
1:F:8:SER:HA	2:G:14:MET:HA	2.00	0.44
1:F:94:LYS:HE3	2:G:152:ASP:OD2	2.18	0.44
3:D:38:TYR:CE2	3:D:57:TYR:HB2	2.53	0.44
4:E:242:LYS:HA	4:E:243:PRO:HD3	1.90	0.43
3:I:127:LYS:HB3	3:I:158:SER:HB3	2.01	0.43
1:F:17:GLY:O	1:F:19:SER:N	2.51	0.43
1:A:8:SER:HA	2:B:14:MET:HA	2.01	0.43
4:E:123:ARG:HE	4:E:167:HIS:CE1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:120:THR:O	2:G:121:ASP:C	2.57	0.43
4:E:8:PRO:HG2	4:E:21:ILE:HA	1.99	0.43
2:B:115:LEU:HD12	2:B:115:LEU:HA	1.91	0.43
3:D:14:TYR:CD1	3:D:127:LYS:HB2	2.54	0.43
1:A:14:GLN:HE21	1:A:19:SER:HB2	1.85	0.42
2:G:73:ALA:O	2:G:77:ARG:HG3	2.18	0.42
1:F:153:LEU:HD22	1:F:161:TYR:CE1	2.54	0.42
2:G:78:VAL:HG11	5:H:4:GLN:HG3	2.02	0.42
1:F:73:LEU:HD12	2:G:53:LEU:HD13	2.02	0.42
1:A:122:LEU:HD23	1:A:127:SER:HA	2.02	0.41
4:E:143:PRO:HD3	4:E:156:LEU:HD13	2.00	0.41
1:A:72:SER:OG	5:C:12:SER:HB3	2.19	0.41
2:B:162:GLU:HB3	2:G:59:GLU:OE2	2.19	0.41
2:B:78:VAL:HG22	5:C:2:PHE:HD2	1.85	0.41
5:C:0:GLN:HB2	5:C:1:PRO:HD3	2.01	0.41
4:E:216:ASN:OD1	4:E:219:ASN:ND2	2.53	0.41
1:F:52:ARG:HA	1:F:52:ARG:HD3	1.90	0.41
1:F:113:PHE:CE1	2:G:34:ARG:HG3	2.55	0.41
2:G:10:GLN:HB2	2:G:31:ILE:HB	2.02	0.41
2:B:46:GLU:OE2	2:G:140:ALA:HB2	2.20	0.41
2:G:26:LEU:HD11	5:H:4:GLN:HE22	1.84	0.41
1:A:140:LYS:HB3	1:A:140:LYS:HE2	1.91	0.41
1:A:15:SER:O	1:A:17:GLY:N	2.53	0.41
1:A:66:LEU:N	1:A:66:LEU:HD23	2.35	0.41
1:F:94:LYS:NZ	2:G:121:ASP:OD1	2.47	0.41
3:D:65:LYS:HD3	3:D:79:PHE:CD1	2.56	0.41
4:J:8:PRO:CD	4:J:21:ILE:HG23	2.51	0.41
5:H:4:GLN:HA	5:H:5:PRO:HD3	1.92	0.40
1:A:14:GLN:CG	1:A:19:SER:HB2	2.51	0.40
4:J:48:GLN:HG2	4:J:49:SER:H	1.86	0.40
1:A:73:LEU:HD12	2:B:53:LEU:HD13	2.02	0.40
2:B:19:ASN:HB3	2:B:22:GLU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	174/183 (95%)	165 (95%)	6 (3%)	3 (2%)	9	36
1	F	176/183 (96%)	166 (94%)	9 (5%)	1 (1%)	25	59
2	B	169/205 (82%)	163 (96%)	6 (4%)	0	100	100
2	G	176/205 (86%)	168 (96%)	7 (4%)	1 (1%)	25	59
3	D	182/203 (90%)	170 (93%)	12 (7%)	0	100	100
3	I	162/203 (80%)	158 (98%)	4 (2%)	0	100	100
4	E	240/246 (98%)	232 (97%)	8 (3%)	0	100	100
4	J	226/246 (92%)	218 (96%)	7 (3%)	1 (0%)	34	69
5	C	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
5	H	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
All	All	1527/1700 (90%)	1460 (96%)	61 (4%)	6 (0%)	34	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	PRO
1	F	18	PRO
1	A	17	GLY
2	G	121	ASP
4	J	144	SER
1	A	16	TYR

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	162/167 (97%)	161 (99%)	1 (1%)	86	94
1	F	162/167 (97%)	159 (98%)	3 (2%)	57	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	161/182 (88%)	161 (100%)	0	100	100
2	G	165/182 (91%)	163 (99%)	2 (1%)	71	88
3	D	169/184 (92%)	162 (96%)	7 (4%)	30	64
3	I	152/184 (83%)	151 (99%)	1 (1%)	84	93
4	E	214/217 (99%)	210 (98%)	4 (2%)	57	81
4	J	204/217 (94%)	203 (100%)	1 (0%)	88	94
5	C	12/12 (100%)	12 (100%)	0	100	100
5	H	12/12 (100%)	12 (100%)	0	100	100
All	All	1413/1524 (93%)	1394 (99%)	19 (1%)	69	87

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	F	18	PRO
1	F	86	VAL
1	F	90	THR
2	G	121	ASP
2	G	143	VAL
3	D	3	LYS
3	D	38	TYR
3	D	65	LYS
3	D	67	THR
3	D	83	ASP
3	D	207	ASN
3	D	209	ILE
4	E	10	ARG
4	E	83	ASN
4	E	130	LEU
4	E	184	CYS
3	I	38	TYR
4	J	183	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
3	I	55	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	NAG	F	201	1	14,14,15	0.54	0	17,19,21	1.21	1 (5%)
7	EDO	J	300	-	3,3,3	0.45	0	2,2,2	0.35	0
7	EDO	J	301	-	3,3,3	0.46	0	2,2,2	0.32	0
7	EDO	A	202	-	3,3,3	0.46	0	2,2,2	0.33	0
8	ACT	F	202	-	1,3,3	6.38	1 (100%)	0,3,3	-	-
8	ACT	A	203	-	1,3,3	3.34	1 (100%)	0,3,3	-	-
6	NAG	A	201	1	14,14,15	0.28	0	17,19,21	0.74	1 (5%)

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	NAG	F	201	1	-	1/6/23/26	0/1/1/1
7	EDO	J	300	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	J	301	-	-	0/1/1/1	-
7	EDO	A	202	-	-	0/1/1/1	-
6	NAG	A	201	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	202	ACT	CH3-C	6.38	1.56	1.48
8	A	203	ACT	CH3-C	3.34	1.53	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	201	NAG	C1-O5-C5	-3.41	107.57	112.19
6	A	201	NAG	C1-O5-C5	2.78	115.95	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	201	NAG	O5-C5-C6-O6
6	A	201	NAG	C4-C5-C6-O6
6	F	201	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	201	NAG	1	0
8	A	203	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	178/183 (97%)	-0.14	5 (2%) 53 30	44, 65, 116, 163	0
1	F	178/183 (97%)	-0.27	0 100 100	34, 52, 91, 128	0
2	B	175/205 (85%)	0.04	6 (3%) 45 24	38, 73, 117, 169	0
2	G	180/205 (87%)	-0.11	0 100 100	38, 60, 101, 135	0
3	D	188/203 (92%)	0.36	11 (5%) 22 10	53, 89, 140, 180	0
3	I	170/203 (83%)	-0.04	1 (0%) 89 78	48, 78, 128, 158	0
4	E	242/246 (98%)	-0.06	1 (0%) 92 84	41, 64, 109, 139	0
4	J	232/246 (94%)	0.01	3 (1%) 77 59	37, 68, 118, 160	0
5	C	13/13 (100%)	-0.23	0 100 100	44, 51, 93, 99	0
5	H	13/13 (100%)	-0.07	0 100 100	42, 50, 77, 90	0
All	All	1569/1700 (92%)	-0.02	27 (1%) 70 49	34, 68, 119, 180	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	156	SER	4.5
4	J	144	SER	3.6
4	J	150	THR	3.5
1	A	157	ALA	3.1
3	D	169	ASP	2.9
3	D	205	PHE	2.9
3	D	161	ASN	2.8
2	B	181	GLN	2.8
3	D	195	ASN	2.8
3	D	207	ASN	2.7
2	B	133	ARG	2.6
3	D	194	SER	2.5
1	A	128	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	203	ASN	2.3
3	I	139	GLN	2.3
3	D	129	ASN	2.3
4	E	209	VAL	2.3
1	A	18	PRO	2.2
2	B	170	VAL	2.2
2	B	135	ASP	2.1
3	D	190	ALA	2.1
2	B	22	GLU	2.1
4	J	151	GLN	2.1
2	B	189	ARG	2.1
3	D	79	PHE	2.0
1	A	161	TYR	2.0
3	D	206	ASN	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	NAG	F	201	14/15	0.54	0.38	61,126,133,135	0
9	CA	E	301	1/1	0.83	0.12	30,30,30,30	0
8	ACT	F	202	4/4	0.84	0.32	55,73,77,84	0
7	EDO	J	300	4/4	0.86	0.17	66,84,84,85	0
7	EDO	A	202	4/4	0.87	0.28	66,68,73,84	0
9	CA	B	201	1/1	0.88	0.23	30,30,30,30	0
8	ACT	A	203	4/4	0.88	0.48	73,78,79,91	0
6	NAG	A	201	14/15	0.91	0.19	61,81,101,102	0
7	EDO	J	301	4/4	0.91	0.16	77,81,81,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.