



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:34 AM UTC

PDB ID : 7Z50 / pdb_00007z50
Title : Structure of the highly diabetogenic 4.1-T cell receptor targeting a hybrid insulin peptide bound to I-Ag7.
Authors : Lopez-Sagaseta, J.; Erausquin, E.
Deposited on : 2022-03-06
Resolution : 2.65 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

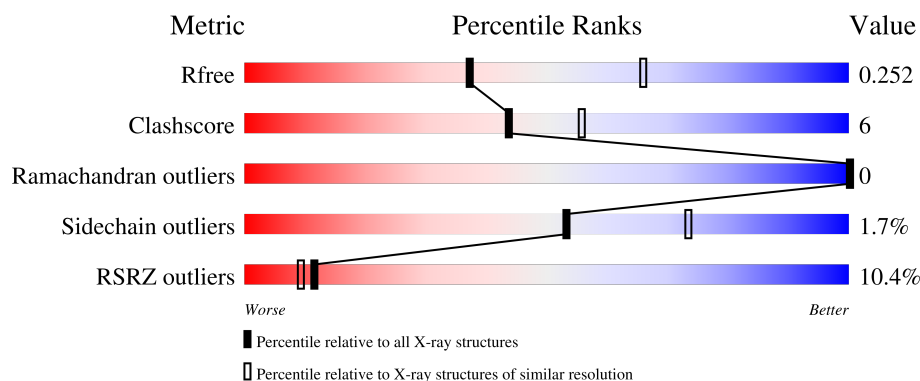
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	202	
1	C	202	
2	B	230	
2	D	230	
3	E	242	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	242	
4	G	207	
4	H	207	
5	T	15	
5	W	15	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12716 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 H-2 class II histocompatibility antigen, A-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1397	902	227	265	3			
1	C	181	Total	C	N	O	S	0	0	0
			1400	909	225	263	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	CYS	ILE	engineered mutation	UNP P04228
A	194	SER	-	expression tag	UNP P04228
A	195	LEU	-	expression tag	UNP P04228
A	196	GLU	-	expression tag	UNP P04228
A	197	VAL	-	expression tag	UNP P04228
A	198	LEU	-	expression tag	UNP P04228
A	199	PHE	-	expression tag	UNP P04228
A	200	GLN	-	expression tag	UNP P04228
C	74	CYS	ILE	engineered mutation	UNP P04228
C	194	SER	-	expression tag	UNP P04228
C	195	LEU	-	expression tag	UNP P04228
C	196	GLU	-	expression tag	UNP P04228
C	197	VAL	-	expression tag	UNP P04228
C	198	LEU	-	expression tag	UNP P04228
C	199	PHE	-	expression tag	UNP P04228
C	200	GLN	-	expression tag	UNP P04228

- Molecule 2 is a protein called H2-Ab1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1437	906	256	269	6			
2	D	173	Total	C	N	O	S	0	0	0
			1369	868	239	256	6			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-25	LEU	-	expression tag	UNP Q31135
B	-24	GLN	-	expression tag	UNP Q31135
B	-23	THR	-	expression tag	UNP Q31135
B	-22	LEU	-	expression tag	UNP Q31135
B	-21	ALA	-	expression tag	UNP Q31135
B	-20	LEU	-	expression tag	UNP Q31135
B	-19	GLU	-	expression tag	UNP Q31135
B	-18	VAL	-	expression tag	UNP Q31135
B	-17	GLU	-	expression tag	UNP Q31135
B	-16	ASP	-	expression tag	UNP Q31135
B	-15	ASP	-	expression tag	UNP Q31135
B	-14	PRO	-	expression tag	UNP Q31135
B	-13	CYS	-	expression tag	UNP Q31135
B	-12	GLY	-	expression tag	UNP Q31135
B	-11	GLY	-	expression tag	UNP Q31135
B	-10	GLY	-	expression tag	UNP Q31135
B	-9	GLY	-	expression tag	UNP Q31135
B	-8	GLY	-	expression tag	UNP Q31135
B	-7	SER	-	expression tag	UNP Q31135
B	-6	GLY	-	expression tag	UNP Q31135
B	-5	GLY	-	expression tag	UNP Q31135
B	-4	GLY	-	expression tag	UNP Q31135
B	-3	SER	-	expression tag	UNP Q31135
B	-2	GLY	-	expression tag	UNP Q31135
B	-1	GLY	-	expression tag	UNP Q31135
B	0	SER	-	expression tag	UNP Q31135
B	198	SER	-	expression tag	UNP Q31135
B	199	LEU	-	expression tag	UNP Q31135
B	200	GLU	-	expression tag	UNP Q31135
B	201	VAL	-	expression tag	UNP Q31135
B	202	LEU	-	expression tag	UNP Q31135
B	203	PHE	-	expression tag	UNP Q31135
B	204	GLN	-	expression tag	UNP Q31135
D	-25	LEU	-	expression tag	UNP Q31135
D	-24	GLN	-	expression tag	UNP Q31135
D	-23	THR	-	expression tag	UNP Q31135
D	-22	LEU	-	expression tag	UNP Q31135
D	-21	ALA	-	expression tag	UNP Q31135
D	-20	LEU	-	expression tag	UNP Q31135
D	-19	GLU	-	expression tag	UNP Q31135
D	-18	VAL	-	expression tag	UNP Q31135
D	-17	GLU	-	expression tag	UNP Q31135

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	ASP	-	expression tag	UNP Q31135
D	-15	ASP	-	expression tag	UNP Q31135
D	-14	PRO	-	expression tag	UNP Q31135
D	-13	CYS	-	expression tag	UNP Q31135
D	-12	GLY	-	expression tag	UNP Q31135
D	-11	GLY	-	expression tag	UNP Q31135
D	-10	GLY	-	expression tag	UNP Q31135
D	-9	GLY	-	expression tag	UNP Q31135
D	-8	GLY	-	expression tag	UNP Q31135
D	-7	SER	-	expression tag	UNP Q31135
D	-6	GLY	-	expression tag	UNP Q31135
D	-5	GLY	-	expression tag	UNP Q31135
D	-4	GLY	-	expression tag	UNP Q31135
D	-3	SER	-	expression tag	UNP Q31135
D	-2	GLY	-	expression tag	UNP Q31135
D	-1	GLY	-	expression tag	UNP Q31135
D	0	SER	-	expression tag	UNP Q31135
D	198	SER	-	expression tag	UNP Q31135
D	199	LEU	-	expression tag	UNP Q31135
D	200	GLU	-	expression tag	UNP Q31135
D	201	VAL	-	expression tag	UNP Q31135
D	202	LEU	-	expression tag	UNP Q31135
D	203	PHE	-	expression tag	UNP Q31135
D	204	GLN	-	expression tag	UNP Q31135

- Molecule 3 is a protein called 4.1 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	242	Total	C	N	O	S	0	0	0
			1855	1175	326	346	8			
3	F	241	Total	C	N	O	S	0	0	0
			1849	1171	323	348	7			

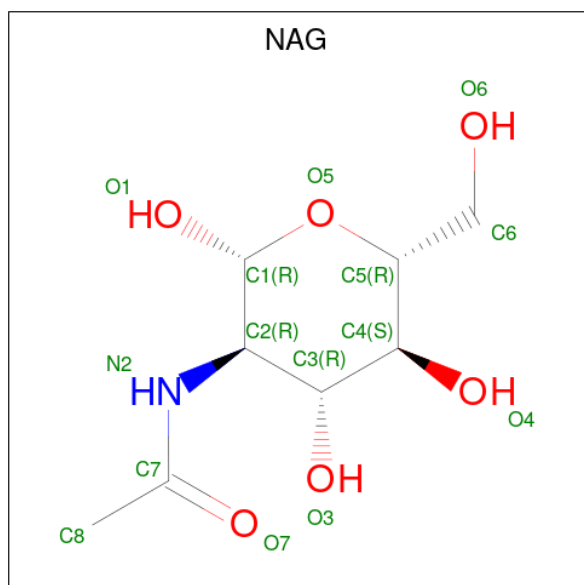
- Molecule 4 is a protein called 4.1 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	185	Total	C	N	O	S	0	0	0
			1382	868	234	272	8			
4	H	186	Total	C	N	O	S	0	0	0
			1391	878	235	270	8			

- Molecule 5 is a protein called Hybrid insulin peptide.

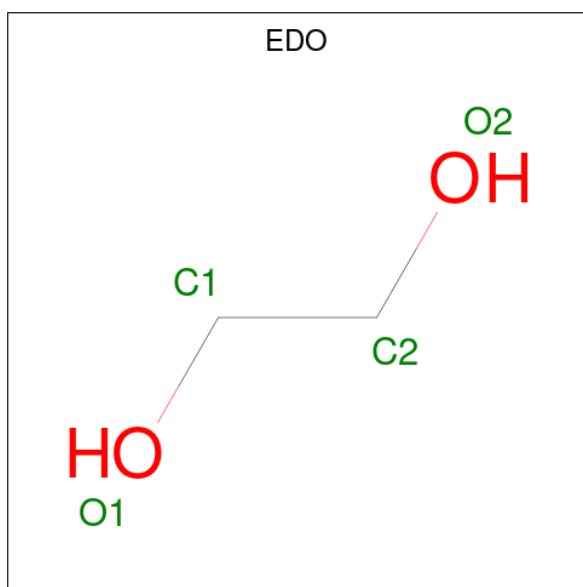
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	T	13	Total 99	C 61	N 14	O 23	S 1	0	0	0
5	W	15	Total 107	C 65	N 16	O 25	S 1	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	G	1	Total	C	O	0	0
			4	2	2		
7	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	1	Total	Na	0	0
			1	1		
8	H	1	Total	Na	0	0
			1	1		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	1	Total	Cl	0	0
			1	1		

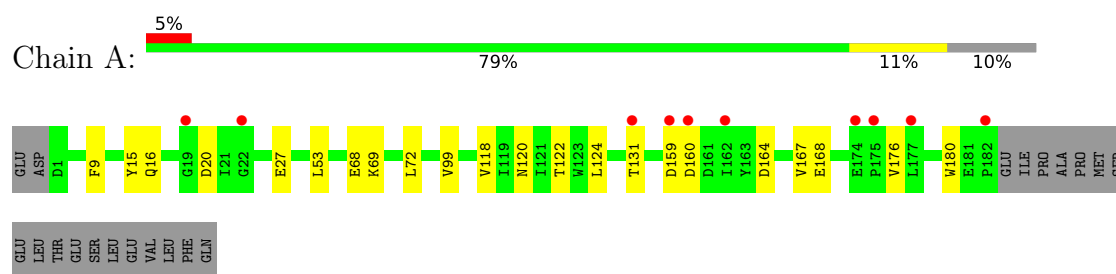
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	33	Total 33	O 33	0	0
10	B	47	Total 47	O 47	0	0
10	C	34	Total 34	O 34	0	0
10	D	41	Total 41	O 41	0	0
10	E	34	Total 34	O 34	0	0
10	F	51	Total 51	O 51	0	0
10	G	33	Total 33	O 33	0	0
10	H	45	Total 45	O 45	0	0
10	T	9	Total 9	O 9	0	0
10	W	6	Total 6	O 6	0	0

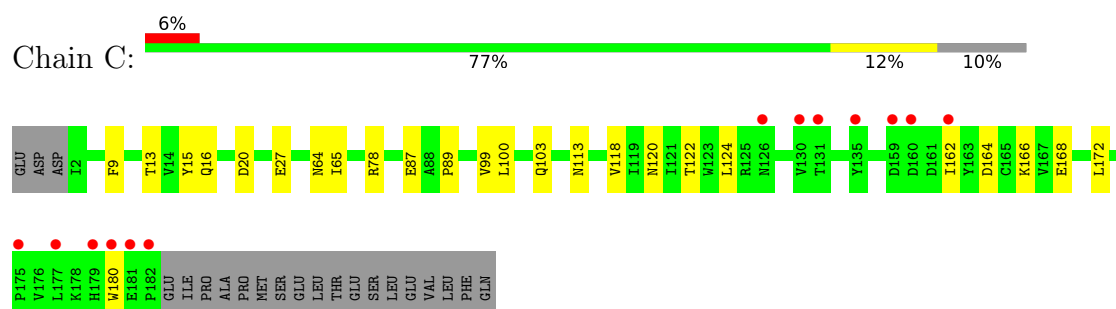
3 Residue-property plots [i](#)

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.

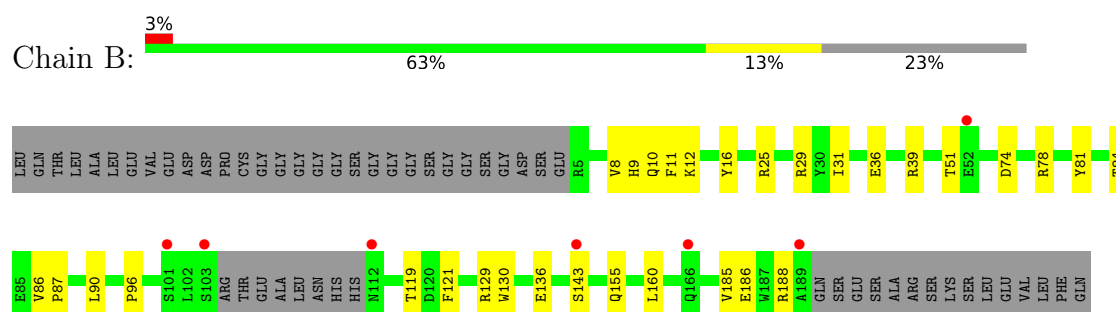
- Molecule 1: H-2 class II histocompatibility antigen, A-D alpha chain



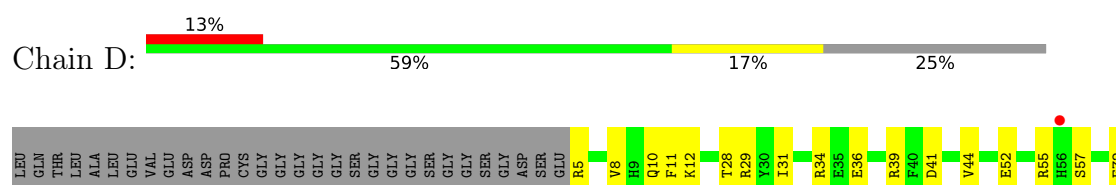
- Molecule 1: H-2 class II histocompatibility antigen, A-D alpha chain



- Molecule 2: H2-Ab1 protein



- Molecule 2: H2-Ab1 protein



- Molecule 5: Hybrid insulin peptide

Chain T:  67% 20% 13%



- Molecule 5: Hybrid insulin peptide

Chain W:  13% 73% 27%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	213.62Å 133.46Å 102.56Å 90.00° 103.69° 90.00°	Depositor
Resolution (Å)	49.82 – 2.65 49.82 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.82-2.65) 99.9 (49.82-2.65)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.221 , 0.261 (Not available) , 0.252	Depositor DCC
R_{free} test set	4064 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtrriage
Anisotropy	0.198	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12716	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4844e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EDO, NAG, NA, CL

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	0.09	0/1442	0.26	0/1981
1	C	0.09	0/1446	0.27	0/1984
2	B	0.12	0/1471	0.29	0/2000
2	D	0.09	0/1401	0.26	0/1908
3	E	0.09	0/1908	0.30	0/2609
3	F	0.08	0/1901	0.26	0/2599
4	G	0.11	0/1409	0.33	0/1916
4	H	0.09	0/1418	0.30	0/1927
5	T	0.08	0/99	0.30	0/135
5	W	0.10	0/107	0.31	0/145
All	All	0.10	0/12602	0.29	0/17204

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	1397	0	1251	16	0
1	C	1400	0	1266	21	0
2	B	1437	0	1341	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1369	0	1247	21	0
3	E	1855	0	1712	22	0
3	F	1849	0	1709	22	0
4	G	1382	0	1251	17	0
4	H	1391	0	1282	20	0
5	T	99	0	95	2	0
5	W	107	0	101	3	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	28	0	26	0	0
6	D	14	0	13	0	0
7	A	4	0	6	0	0
7	B	4	0	6	0	0
7	D	4	0	6	0	0
7	E	4	0	6	0	0
7	G	8	0	12	1	0
8	F	1	0	0	0	0
8	H	1	0	0	0	0
9	G	1	0	0	0	0
10	A	33	0	0	0	0
10	B	47	0	0	0	0
10	C	34	0	0	3	0
10	D	41	0	0	2	0
10	E	34	0	0	2	0
10	F	51	0	0	1	0
10	G	33	0	0	2	0
10	H	45	0	0	2	0
10	T	9	0	0	0	0
10	W	6	0	0	0	0
All	All	12716	0	11356	144	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 6.

All (144) 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:15:TYR:OH	1:A:20:ASP:OD1	1.94	0.85
2:D:98:VAL:HG21	2:D:174:VAL:HG11	1.64	0.80
3:E:166:SER:OG	4:H:164:MET:O	2.03	0.76
1:C:13:THR:OG1	10:C:401:HOH:O	2.05	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:ASP:OD1	2:D:78:ARG:NH1	2.24	0.71
2:B:74:ASP:OD1	2:B:78:ARG:NE	2.27	0.68
2:D:52:GLU:OE1	2:D:55:ARG:NH1	2.27	0.67
1:A:124:LEU:HB2	1:A:164:ASP:HB2	1.78	0.66
3:F:193:ARG:NH1	10:F:403:HOH:O	2.28	0.65
4:H:46:LYS:NZ	10:H:404:HOH:O	2.30	0.65
3:F:29:SER:OG	5:W:8:ASP:OD2	2.15	0.64
3:F:130:GLU:OE1	4:G:125:ARG:NH1	2.30	0.64
3:F:138:LYS:HD3	4:G:164:MET:HE1	1.79	0.63
2:D:5:ARG:N	10:D:403:HOH:O	2.33	0.61
3:E:1:MET:SD	3:E:1:MET:N	2.71	0.61
3:E:33:TRP:HB2	3:E:46:THR:HG22	1.82	0.61
4:G:28:ASP:OD2	7:G:303:EDO:O2	2.18	0.61
1:C:87:GLU:OE2	2:D:34:ARG:NH1	2.33	0.61
1:C:124:LEU:HB2	1:C:164:ASP:HB2	1.84	0.60
1:C:16:GLN:HG2	2:D:8:VAL:HG22	1.81	0.60
2:D:10:GLN:HB2	2:D:31:ILE:HB	1.83	0.60
3:F:132:GLU:OE2	3:F:193:ARG:NH2	2.35	0.59
3:F:20:LEU:HD22	3:F:107:THR:HG21	1.84	0.59
1:C:120:ASN:HB2	1:C:168:GLU:HB2	1.85	0.58
1:C:13:THR:HG23	1:C:65:ILE:HD13	1.85	0.57
3:E:138:LYS:HD3	4:H:164:MET:HE1	1.84	0.57
1:C:16:GLN:HE22	1:C:118:VAL:HG23	1.70	0.57
1:C:64:ASN:ND2	10:C:401:HOH:O	2.17	0.56
4:G:144:THR:O	4:G:159:LYS:NZ	2.35	0.56
2:D:100:ILE:HD11	2:D:172:CYS:HB2	1.88	0.55
3:E:35:ARG:NH1	3:E:43:GLU:OE1	2.39	0.55
1:A:68:GLU:OE1	2:B:9:HIS:ND1	2.38	0.55
3:E:116:LYS:O	10:E:401:HOH:O	2.17	0.55
2:B:119:THR:HG22	2:B:155:GLN:HB2	1.89	0.54
1:C:15:TYR:OH	1:C:20:ASP:OD1	2.20	0.54
2:B:186:GLU:OE1	2:B:188:ARG:NH1	2.35	0.53
4:G:58:LYS:NZ	10:G:404:HOH:O	2.40	0.53
4:H:58:LYS:NZ	10:H:408:HOH:O	2.37	0.52
2:D:41:ASP:HB3	2:D:44:VAL:HG23	1.90	0.52
1:A:120:ASN:HB2	1:A:168:GLU:HB2	1.89	0.52
2:B:11:PHE:CG	5:T:6:VAL:HG22	2.45	0.52
4:H:147:SER:OG	4:H:150:LYS:N	2.42	0.52
2:B:10:GLN:HB2	2:B:31:ILE:HB	1.90	0.52
2:D:95:GLN:NE2	2:D:178:SER:O	2.41	0.51
3:E:34:TYR:OH	4:H:100:TYR:HB2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:51:GLN:NE2	10:E:404:HOH:O	2.44	0.51
1:C:113:ASN:ND2	10:C:405:HOH:O	2.36	0.51
3:F:169:CYS:HB2	4:G:162:LEU:HB3	1.93	0.50
2:B:12:LYS:HB2	2:B:29:ARG:HB2	1.93	0.50
4:H:21:SER:HG	4:H:77:HIS:HD1	1.55	0.50
2:B:86:VAL:HG22	2:B:87:PRO:HD3	1.95	0.49
1:C:9:PHE:HB2	1:C:27:GLU:HB2	1.93	0.49
1:A:16:GLN:HE22	1:A:118:VAL:HG23	1.78	0.49
2:D:11:PHE:CG	5:W:6:VAL:HG22	2.48	0.49
1:A:167:VAL:HB	1:A:176:VAL:HG22	1.95	0.49
4:H:60:THR:O	4:H:60:THR:OG1	2.31	0.49
4:G:161:VAL:HG22	4:G:172:ASN:OD1	2.13	0.49
3:E:29:SER:OG	5:T:8:ASP:OD2	2.28	0.48
4:H:21:SER:OG	4:H:77:HIS:ND1	2.46	0.48
3:F:32:PHE:HB2	3:F:92:ALA:HB3	1.94	0.48
4:H:55:MET:HE1	4:H:58:LYS:HB2	1.94	0.48
4:H:147:SER:HG	4:H:150:LYS:N	2.11	0.48
2:D:36:GLU:OE2	2:D:39:ARG:HB2	2.14	0.47
1:C:89:PRO:HD2	1:C:172:LEU:HG	1.96	0.47
3:F:34:TYR:OH	4:G:100:TYR:HB2	2.14	0.47
3:F:108:ARG:HG2	3:F:152:HIS:CE1	2.49	0.47
4:H:46:LYS:HB2	4:H:46:LYS:HE2	1.56	0.47
3:F:141:LEU:HD13	3:F:192:LEU:HD23	1.97	0.47
1:A:16:GLN:HE22	1:A:118:VAL:CG2	2.28	0.46
2:B:81:TYR:O	2:B:86:VAL:HG13	2.15	0.46
4:H:15:GLN:HG3	4:H:16:GLU:N	2.30	0.46
1:A:9:PHE:HB2	1:A:27:GLU:HB2	1.97	0.46
1:A:99:VAL:HG21	1:A:180:TRP:CZ2	2.51	0.46
3:F:152:HIS:HB3	3:F:213:TYR:HB2	1.97	0.46
4:H:164:MET:C	4:H:166:SER:H	2.25	0.45
2:B:130:TRP:HB3	2:B:160:LEU:HD22	1.98	0.45
3:F:191:ARG:HE	4:G:173:SER:HB2	1.81	0.45
3:F:128:PRO:HD2	3:F:199:TRP:CZ2	2.52	0.45
3:E:115:LEU:O	3:E:118:VAL:HG12	2.17	0.45
1:C:100:LEU:HB2	1:C:103:GLN:HG2	1.97	0.45
2:D:12:LYS:HB2	2:D:29:ARG:HB2	1.98	0.45
4:G:173:SER:OG	10:G:401:HOH:O	2.21	0.45
1:C:99:VAL:HG21	1:C:180:TRP:CZ2	2.52	0.45
1:A:15:TYR:CE1	1:A:69:LYS:HE3	2.51	0.45
2:B:129:ARG:HD2	2:B:136:GLU:OE2	2.17	0.45
2:B:86:VAL:HA	2:B:90:LEU:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:207:ARG:HG3	3:F:236:GLU:HB3	1.99	0.44
1:A:72:LEU:HD13	2:B:9:HIS:HB2	1.99	0.44
3:E:30:ALA:HB1	3:E:47:TYR:HE1	1.82	0.44
3:F:125:VAL:HG13	3:F:235:ALA:HB3	1.99	0.44
2:B:96:PRO:HB3	2:B:121:PHE:HB3	1.99	0.44
1:C:103:GLN:O	1:C:103:GLN:NE2	2.51	0.43
1:C:122:THR:HG23	1:C:166:LYS:HB3	2.00	0.43
4:G:49:ILE:HD13	4:G:65:VAL:HG13	2.00	0.43
2:D:119:THR:HG22	2:D:155:GLN:HB2	2.00	0.43
3:E:120:PRO:HD3	3:E:228:PRO:HB3	1.99	0.43
3:E:221:TRP:NE1	3:E:223:GLN:O	2.52	0.43
3:F:108:ARG:NH2	3:F:151:ASP:HB3	2.34	0.43
1:A:159:ASP:OD1	1:A:160:ASP:N	2.52	0.43
2:B:16:TYR:HB2	2:B:25:ARG:HB3	2.00	0.43
3:E:44:PHE:O	3:E:58:GLY:HA3	2.19	0.43
4:G:124:LEU:HD13	4:G:134:VAL:HG12	2.01	0.43
2:B:36:GLU:O	2:B:51:THR:HG23	2.19	0.43
2:B:84:THR:C	2:B:87:PRO:HD2	2.43	0.43
1:C:100:LEU:O	1:C:103:GLN:HG3	2.19	0.42
2:D:159:MET:SD	2:D:159:MET:N	2.92	0.42
3:E:201:ASN:O	3:E:239:GLY:HA3	2.19	0.42
3:E:96:GLN:HB2	3:E:99:ASN:HB3	2.00	0.42
3:F:30:ALA:HB1	3:F:47:TYR:HE1	1.84	0.42
4:G:127:SER:C	4:G:129:SER:H	2.27	0.42
2:D:151:ASP:OD1	2:D:153:THR:OG1	2.34	0.42
4:H:147:SER:HB3	4:H:156:ILE:HD13	2.01	0.42
2:B:36:GLU:OE2	2:B:39:ARG:HB2	2.20	0.42
4:G:34:PHE:HB2	4:G:51:ILE:HG22	2.01	0.42
4:G:57:ARG:HE	4:G:59:GLN:HE21	1.66	0.42
4:G:154:VAL:HG22	4:G:178:SER:HB2	2.02	0.42
3:E:129:SER:O	3:E:133:ILE:HG13	2.19	0.42
3:E:169:CYS:HB2	4:H:162:LEU:HB3	2.02	0.42
4:H:154:VAL:HG22	4:H:178:SER:HB2	2.01	0.42
1:A:20:ASP:OD1	1:A:69:LYS:HE2	2.19	0.42
3:E:128:PRO:HG2	3:E:139:ALA:HB1	2.02	0.41
3:F:151:ASP:OD1	3:F:174:PRO:HG3	2.20	0.41
3:E:67:GLN:NE2	3:E:75:THR:OG1	2.53	0.41
1:C:99:VAL:HG21	1:C:180:TRP:CH2	2.54	0.41
4:G:111:ILE:HG21	4:G:142:SER:HB3	2.01	0.41
4:H:51:ILE:HG13	4:H:55:MET:HE2	2.01	0.41
3:E:8:ARG:HH12	3:E:105:ALA:HB1	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:49:ARG:HB3	3:F:54:ILE:CD1	2.51	0.41
3:F:128:PRO:HG2	3:F:139:ALA:HB1	2.03	0.41
4:H:34:PHE:HB2	4:H:51:ILE:HG22	2.03	0.41
1:A:15:TYR:CE2	1:A:69:LYS:HG3	2.56	0.41
1:A:16:GLN:HG2	2:B:8:VAL:HG22	2.03	0.41
1:C:162:ILE:HD12	1:C:162:ILE:O	2.20	0.41
2:D:96:PRO:HB3	2:D:121:PHE:HB3	2.02	0.41
3:E:189:SER:OG	3:E:191:ARG:NH1	2.54	0.41
2:D:114:LEU:HD11	2:D:170:TYR:CD1	2.55	0.40
4:H:58:LYS:HB3	4:H:65:VAL:HG23	2.03	0.40
1:C:78:ARG:HD3	5:W:12:GLY:O	2.22	0.40
2:D:72:GLU:HA	2:D:75:THR:OG1	2.21	0.40
3:F:63:ARG:HD2	3:F:79:GLN:O	2.21	0.40
2:D:128:VAL:HA	2:D:173:HIS:O	2.21	0.40
1:A:15:TYR:CZ	1:A:69:LYS:HG3	2.56	0.40
1:C:16:GLN:HE22	1:C:118:VAL:CG2	2.32	0.40
2:D:140:GLY:N	10:D:406:HOH:O	2.38	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	180/202 (89%)	177 (98%)	3 (2%)	0	100	100
1	C	179/202 (89%)	176 (98%)	3 (2%)	0	100	100
2	B	173/230 (75%)	171 (99%)	2 (1%)	0	100	100
2	D	167/230 (73%)	164 (98%)	3 (2%)	0	100	100
3	E	240/242 (99%)	236 (98%)	4 (2%)	0	100	100
3	F	239/242 (99%)	234 (98%)	5 (2%)	0	100	100
4	G	181/207 (87%)	169 (93%)	12 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	182/207 (88%)	172 (94%)	10 (6%)	0	100	100
5	T	11/15 (73%)	11 (100%)	0	0	100	100
5	W	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
All	All	1565/1792 (87%)	1522 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	144/183 (79%)	141 (98%)	3 (2%)	47	69
1	C	145/183 (79%)	145 (100%)	0	100	100
2	B	151/201 (75%)	149 (99%)	2 (1%)	61	77
2	D	139/201 (69%)	137 (99%)	2 (1%)	59	76
3	E	189/210 (90%)	186 (98%)	3 (2%)	55	74
3	F	188/210 (90%)	183 (97%)	5 (3%)	39	61
4	G	140/185 (76%)	137 (98%)	3 (2%)	47	69
4	H	143/185 (77%)	141 (99%)	2 (1%)	59	76
5	T	12/12 (100%)	11 (92%)	1 (8%)	10	18
5	W	12/12 (100%)	11 (92%)	1 (8%)	10	18
All	All	1263/1582 (80%)	1241 (98%)	22 (2%)	53	73

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	122	THR
1	A	131	THR
2	B	143	SER
2	B	185	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	28	THR
2	D	57	SER
3	E	19	THR
3	E	134	SER
3	E	189	SER
3	F	19	THR
3	F	26	SER
3	F	46	THR
3	F	81	THR
3	F	197	THR
4	G	59	GLN
4	G	94	SER
4	G	173	SER
4	H	65	VAL
4	H	173	SER
5	T	11	CYS
5	W	11	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	113	ASN
1	A	142	ASN
1	C	16	GLN
1	C	113	ASN
1	C	142	ASN
2	D	145	GLN
2	D	149	ASN
3	E	51	GLN
3	E	67	GLN
3	E	73	HIS
3	E	98	GLN
3	F	51	GLN
3	F	117	ASN
3	F	137	GLN
3	F	218	ASN
4	G	7	GLN
4	G	59	GLN
4	G	82	GLN
4	H	15	GLN
4	H	32	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	H	115	GLN
4	H	116	ASN
4	H	187	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	$\# Z > 2$
7	EDO	A	302	-	3,3,3	0.42	0	2,2,2	0.40	0
7	EDO	G	303	-	3,3,3	0.43	0	2,2,2	0.35	0
6	NAG	B	301	2	14,14,15	0.27	0	17,19,21	0.45	0
6	NAG	D	301	2	14,14,15	0.29	0	17,19,21	0.39	0
7	EDO	E	301	-	3,3,3	0.43	0	2,2,2	0.38	0
7	EDO	D	302	-	3,3,3	0.43	0	2,2,2	0.39	0
6	NAG	A	301	1	14,14,15	0.24	0	17,19,21	0.46	0
7	EDO	B	302	-	3,3,3	0.42	0	2,2,2	0.38	0
7	EDO	G	301	-	3,3,3	0.43	0	2,2,2	0.41	0
6	NAG	C	301	1	14,14,15	0.58	0	17,19,21	0.50	0
6	NAG	C	302	1	14,14,15	0.29	0	17,19,21	0.52	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
7	EDO	A	302	-	-	0/1/1/1	-
7	EDO	G	303	-	-	0/1/1/1	-
6	NAG	B	301	2	-	0/6/23/26	0/1/1/1
6	NAG	D	301	2	-	1/6/23/26	0/1/1/1
7	EDO	E	301	-	-	0/1/1/1	-
7	EDO	D	302	-	-	0/1/1/1	-
6	NAG	A	301	1	-	2/6/23/26	0/1/1/1
7	EDO	B	302	-	-	0/1/1/1	-
7	EDO	G	301	-	-	0/1/1/1	-
6	NAG	C	301	1	-	0/6/23/26	0/1/1/1
6	NAG	C	302	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	NAG	O5-C5-C6-O6
6	C	302	NAG	O5-C5-C6-O6
6	A	301	NAG	C4-C5-C6-O6
6	C	302	NAG	C4-C5-C6-O6
6	D	301	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	303	EDO	1	0

5.7 Other polymers ⓘ

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, 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	182/202 (90%)	0.39	10 (5%)	30	24	41, 54, 85, 113	0
1	C	181/202 (89%)	0.44	13 (7%)	21	16	41, 57, 84, 116	0
2	B	177/230 (76%)	0.32	7 (3%)	42	34	42, 54, 79, 103	0
2	D	173/230 (75%)	0.73	30 (17%)	4	3	42, 58, 97, 127	0
3	E	242/242 (100%)	0.58	18 (7%)	20	15	46, 68, 107, 122	0
3	F	241/242 (99%)	0.43	15 (6%)	26	20	47, 61, 82, 110	0
4	G	185/207 (89%)	1.05	35 (18%)	3	2	43, 61, 99, 124	0
4	H	186/207 (89%)	1.14	36 (19%)	3	2	43, 69, 104, 148	0
5	T	13/15 (86%)	-0.09	0	100	100	43, 46, 54, 61	0
5	W	15/15 (100%)	0.35	2 (13%)	7	6	44, 46, 87, 90	0
All	All	1595/1792 (89%)	0.62	166 (10%)	11	9	41, 60, 97, 148	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	146	VAL	7.3
4	G	182	ASP	6.3
4	H	182	ASP	5.5
2	D	164	PRO	5.1
4	H	145	ASN	4.9
4	G	128	LYS	4.9
3	E	181	LEU	4.8
4	H	147	SER	4.8
4	G	126	ASP	4.8
4	H	191	ASN	4.7
4	H	186	ALA	4.6
3	E	73	HIS	4.3
4	G	166	SER	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	G	41	PRO	4.3
3	F	62	GLU	4.1
3	F	241	ALA	4.0
4	G	188	ALA	4.0
1	A	160	ASP	3.9
1	A	175	PRO	3.9
2	D	163	THR	3.9
4	H	188	ALA	3.8
4	H	166	SER	3.8
4	G	186	ALA	3.8
1	A	182	PRO	3.8
1	C	131	THR	3.7
1	A	19	GLY	3.7
4	G	168	ASP	3.7
4	G	152	SER	3.6
4	H	153	ASP	3.6
2	B	166	GLN	3.6
4	G	112	ALA	3.6
3	F	182	ASN	3.6
2	B	189	ALA	3.5
2	B	52	GLU	3.5
1	C	182	PRO	3.5
4	G	133	SER	3.4
3	E	218	ASN	3.4
4	G	131	ASP	3.4
4	G	179	ASN	3.4
5	W	13	GLY	3.4
2	D	170	TYR	3.4
2	D	172	CYS	3.4
1	C	181	GLU	3.4
1	C	162	ILE	3.3
2	D	101	SER	3.3
4	H	142	SER	3.3
3	E	242	ASP	3.3
4	G	153	ASP	3.3
3	E	223	GLN	3.3
1	A	159	ASP	3.2
4	G	113	ASP	3.2
4	G	151	ASP	3.2
2	D	113	THR	3.2
3	E	203	ARG	3.1
2	D	136	GLU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	217	GLU	3.1
3	E	222	THR	3.1
4	H	144	THR	3.1
4	H	189	PHE	3.1
4	H	113	ASP	3.1
4	H	128	LYS	3.0
4	G	187	ASN	3.0
1	C	180	TRP	3.0
2	D	103	SER	3.0
4	G	165	ARG	3.0
2	D	167	GLY	3.0
1	C	160	ASP	2.9
4	G	148	GLN	2.9
2	D	138	THR	2.9
3	F	195	SER	2.9
4	H	41	PRO	2.8
2	D	173	HIS	2.8
4	G	146	VAL	2.8
4	H	54	ASN	2.8
4	G	42	GLY	2.8
1	A	131	THR	2.8
1	C	179	HIS	2.8
4	H	151	ASP	2.8
1	C	130	VAL	2.8
3	E	139	ALA	2.8
4	H	114	ILE	2.7
3	E	179	PRO	2.7
4	H	143	GLN	2.7
3	E	119	PHE	2.7
1	C	135	TYR	2.7
3	E	195	SER	2.7
4	G	147	SER	2.7
4	H	159	LYS	2.7
4	G	4	GLN	2.6
3	F	178	GLN	2.6
4	G	167	MET	2.6
4	G	73	ARG	2.6
4	G	170	LYS	2.6
2	D	133	ASN	2.6
2	D	143	SER	2.6
2	D	169	VAL	2.6
3	F	181	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	174	GLU	2.6
3	F	137	GLN	2.6
4	H	112	ALA	2.5
1	C	159	ASP	2.5
3	F	180	ALA	2.5
4	H	131	ASP	2.5
2	D	100	ILE	2.5
3	E	224	ASP	2.5
2	D	115	VAL	2.5
3	F	71	GLN	2.5
4	H	133	SER	2.4
3	E	183	ASP	2.4
5	W	12	GLY	2.4
3	F	197	THR	2.4
1	C	126	ASN	2.4
4	G	178	SER	2.4
1	C	175	PRO	2.4
4	H	70	LYS	2.4
4	G	132	LYS	2.4
1	A	22	GLY	2.4
4	H	183	PHE	2.4
3	F	114	ASP	2.4
4	G	115	GLN	2.4
2	D	139	VAL	2.4
2	B	101	SER	2.3
4	H	152	SER	2.3
2	D	174	VAL	2.3
2	D	160	LEU	2.3
2	D	128	VAL	2.3
3	F	1	MET	2.3
4	H	115	GLN	2.3
2	D	187	TRP	2.3
1	A	177	LEU	2.3
2	D	102	LEU	2.3
4	G	111	ILE	2.2
3	F	61	LYS	2.2
4	H	164	MET	2.2
3	E	202	PRO	2.2
4	H	181	SER	2.2
3	E	12	THR	2.2
3	E	182	ASN	2.2
1	C	177	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	103	SER	2.2
2	B	143	SER	2.2
4	H	120	ALA	2.2
3	F	46	THR	2.2
4	G	80	ASP	2.2
2	D	181	SER	2.2
1	A	162	ILE	2.2
2	D	130	TRP	2.1
4	H	150	LYS	2.1
4	H	126	ASP	2.1
4	G	127	SER	2.1
4	H	118	ASP	2.1
4	H	53	SER	2.1
3	F	235	ALA	2.1
2	D	129	ARG	2.1
2	B	112	ASN	2.1
4	G	40	GLU	2.1
4	G	143	GLN	2.1
2	D	179	LEU	2.1
4	H	177	TRP	2.0
2	D	114	LEU	2.0
3	E	173	GLN	2.0
2	D	56	HIS	2.0
2	D	112	ASN	2.0
4	G	134	VAL	2.0
2	D	132	ARG	2.0
4	H	116	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 oligosaccharides 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	D	301	14/15	0.46	0.22	101,119,136,140	0
6	NAG	C	301	14/15	0.67	0.17	90,97,108,109	0
6	NAG	A	301	14/15	0.72	0.17	75,97,101,103	0
6	NAG	C	302	14/15	0.77	0.16	79,102,109,109	0
6	NAG	B	301	14/15	0.78	0.15	84,94,101,103	0
7	EDO	G	303	4/4	0.79	0.28	59,59,61,65	0
7	EDO	B	302	4/4	0.89	0.17	53,57,59,59	0
7	EDO	A	302	4/4	0.89	0.12	54,58,58,62	0
7	EDO	E	301	4/4	0.90	0.17	67,68,71,74	0
7	EDO	G	301	4/4	0.91	0.11	50,52,54,59	0
7	EDO	D	302	4/4	0.94	0.12	64,65,71,72	0
8	NA	F	301	1/1	0.96	0.19	47,47,47,47	1
8	NA	H	301	1/1	0.97	0.17	47,47,47,47	0
9	CL	G	302	1/1	0.97	0.05	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.