



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:02 PM UTC

PDB ID : 8VD0 / pdb_00008vd0
Title : Human TCR ET650-4 in complex with DQ8-InsC8-15-IAPP2
Authors : Tran, T.M.; Lim, J.J.; Loh, T.Y.; Mannering, I.S.; Rossjohn, J.; Reid, H.H.
Deposited on : 2023-12-14
Resolution : 2.40 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

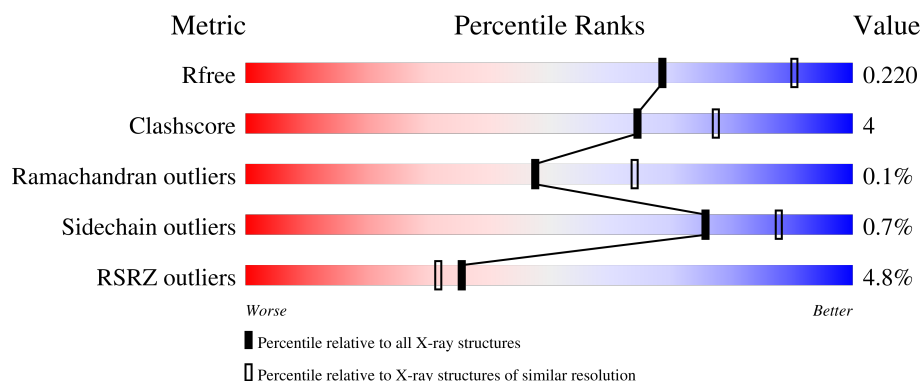
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	185	2% 91% 7% ..
1	F	185	4% 90% 8% .
2	C	213	5% 77% 14% 9%
2	H	213	8% 79% 12% 8%
3	D	206	6% 90% 8% .

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Mol	Chain	Length	Quality of chain
3	I	206	9% 93%
4	E	240	2% 90% 10%
4	J	240	2% 89% 11%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13282 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 MHC class II HLA-DQ-alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1464	944	242	275	3			
1	F	180	Total	C	N	O	S	0	0	0
			1436	926	238	269	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	CYS	ILE	engineered mutation	UNP Q30069
F	72	CYS	ILE	engineered mutation	UNP Q30069

- Molecule 2 is a protein called Hybrid insulin peptide (HIP; InsC8-15-IAPP74-80),MHC class II HLA-DQ-beta-1 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	194	Total	C	N	O	S	0	0	0
			1521	965	262	286	8			
2	H	195	Total	C	N	O	S	0	0	0
			1509	958	262	283	6			

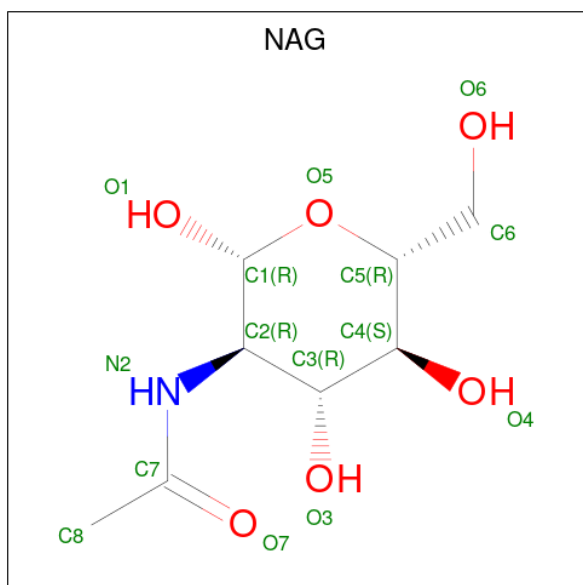
- Molecule 3 is a protein called T-CELL-RECEPTOR, TCR ET650-4 alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	202	Total	C	N	O	S	0	0	0
			1524	953	257	304	10			
3	I	201	Total	C	N	O	S	0	0	0
			1490	937	248	294	11			

- Molecule 4 is a protein called T-CELL-RECEPTOR, TCR ET650-4 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	240	Total	C	N	O	S	0	0	0
			1897	1196	337	358	6			
4	J	240	Total	C	N	O	S	0	0	0
			1895	1195	335	359	6			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	I	1	Total	C	O	0	0
			6	3	3		
6	J	1	Total	C	O	0	0
			6	3	3		
6	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		
7	C	1	Total	O	P	0	0
			5	4	1		
7	D	1	Total	O	P	0	0
			5	4	1		
7	E	1	Total	O	P	0	0
			5	4	1		
7	I	1	Total	O	P	0	0
			5	4	1		
7	J	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	50	Total	O	0	0
			50	50		
8	C	39	Total	O	0	0
			39	39		
8	F	32	Total	O	0	0
			32	32		
8	H	28	Total	O	0	0
			28	28		
8	D	51	Total	O	0	0
			51	51		
8	E	80	Total	O	0	0
			80	80		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	43	Total 43	O 43	0	0
8	J	51	Total 51	O 51	0	0

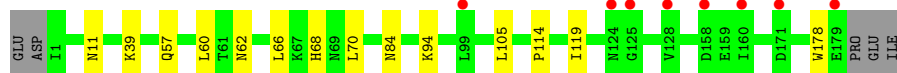
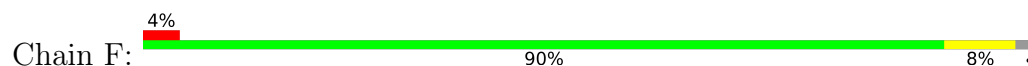
3 Residue-property plots

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.

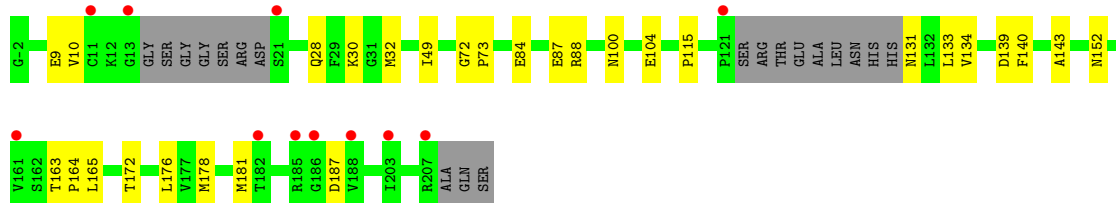
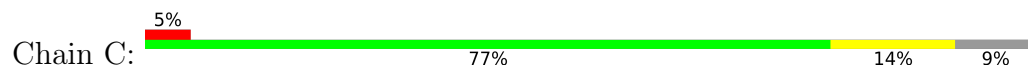
- Molecule 1: MHC class II HLA-DQ-alpha chain



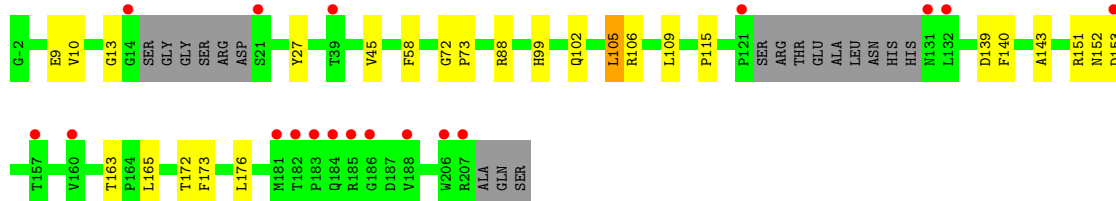
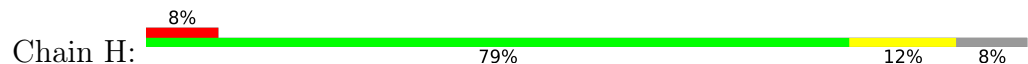
- Molecule 1: MHC class II HLA-DQ-alpha chain



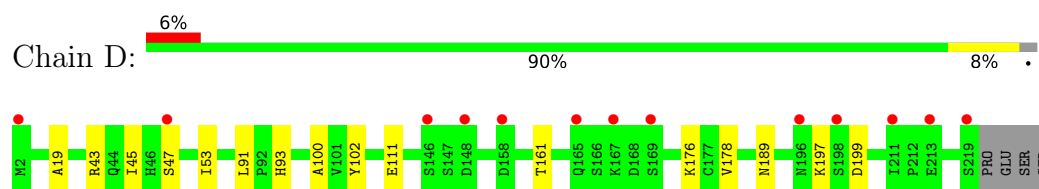
- Molecule 2: Hybrid insulin peptide (HIP; InsC8-15-IAPP74-80),MHC class II HLA-DQ-beta-1 chimera



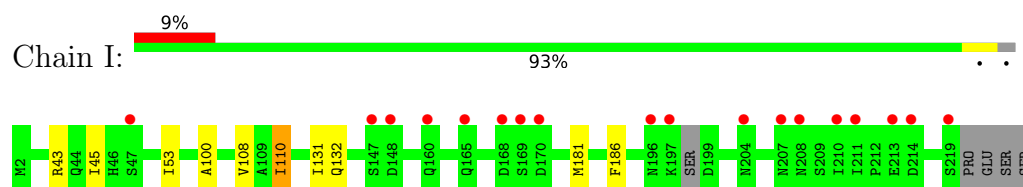
- Molecule 2: Hybrid insulin peptide (HIP; InsC8-15-IAPP74-80),MHC class II HLA-DQ-beta-1 chimera



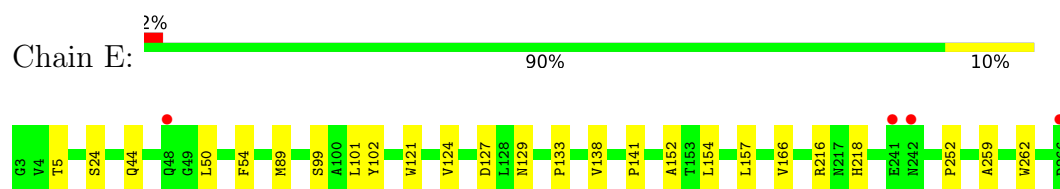
- Molecule 3: T-CELL-RECEPTOR, TCR ET650-4 alpha



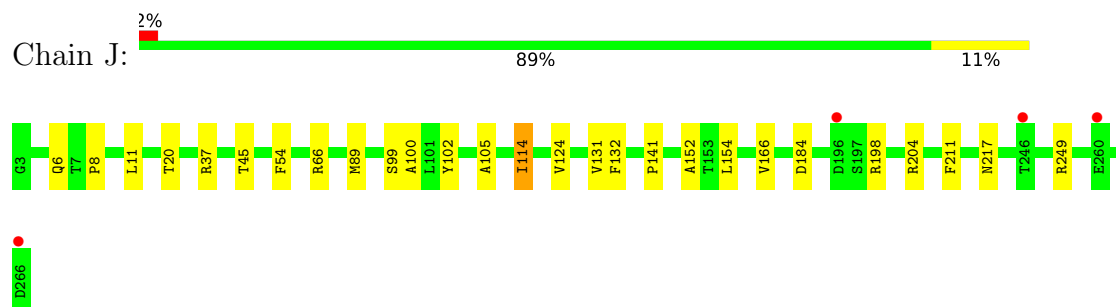
- Molecule 3: T-CELL-RECEPTOR, TCR ET650-4 alpha



- Molecule 4: T-CELL-RECEPTOR, TCR ET650-4 beta



- Molecule 4: T-CELL-RECEPTOR, TCR ET650-4 beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.19Å 139.30Å 120.50Å 90.00° 93.70° 90.00°	Depositor
Resolution (Å)	45.51 – 2.40 45.51 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.51-2.40) 98.6 (45.51-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.188 , 0.220 0.188 , 0.220	Depositor DCC
R_{free} test set	4596 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13282	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, PO4

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	0.11	0/1508	0.29	0/2060
1	F	0.10	0/1479	0.26	0/2019
2	C	0.11	0/1556	0.32	0/2124
2	H	0.11	0/1544	0.33	0/2109
3	D	0.10	0/1557	0.27	0/2124
3	I	0.10	0/1522	0.26	0/2077
4	E	0.11	0/1949	0.29	0/2652
4	J	0.10	0/1947	0.28	0/2650
All	All	0.11	0/13062	0.29	0/17815

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1464	0	1394	8	0
1	F	1436	0	1362	12	0
2	C	1521	0	1421	19	0
2	H	1509	0	1400	18	0
3	D	1524	0	1414	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1490	0	1364	7	0
4	E	1897	0	1792	14	0
4	J	1895	0	1787	15	0
5	A	28	0	26	0	0
5	F	28	0	26	0	0
5	H	14	0	13	0	0
6	A	12	0	16	0	0
6	D	6	0	8	0	0
6	E	6	0	8	0	0
6	F	18	0	24	4	0
6	H	6	0	8	2	0
6	I	12	0	16	3	0
6	J	12	0	16	2	0
7	A	5	0	0	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
7	E	5	0	0	0	0
7	I	5	0	0	0	0
7	J	5	0	0	0	0
8	A	50	0	0	1	0
8	C	39	0	0	2	0
8	D	51	0	0	0	0
8	E	80	0	0	0	0
8	F	32	0	0	1	0
8	H	28	0	0	1	0
8	I	43	0	0	2	0
8	J	51	0	0	0	0
All	All	13282	0	12095	97	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 4.

All (97) 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:119:ILE:H	6:F:204:GOL:H31	1.46	0.80
2:H:13:GLY:O	4:J:37:ARG:NH1	2.28	0.67
2:C:84:GLU:OE2	2:C:88:ARG:NH1	2.27	0.67
2:C:134:VAL:HG22	2:C:178:MET:HG3	1.77	0.67
2:H:143:ALA:HB1	2:H:165:LEU:HD21	1.80	0.63
1:A:11:ASN:HD21	1:A:62:ASN:HD22	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:163:THR:HG22	2:H:176:LEU:H	1.67	0.60
3:I:186:PHE:HA	6:I:302:GOL:H12	1.85	0.59
3:I:131:ILE:HA	6:I:302:GOL:H31	1.86	0.58
1:F:11:ASN:HD21	1:F:62:ASN:HD22	1.52	0.57
2:H:88:ARG:NH2	8:H:401:HOH:O	2.36	0.57
3:I:108:VAL:HB	3:I:110:ILE:HD12	1.85	0.57
4:J:105:ALA:HB1	4:J:114:ILE:HG23	1.86	0.56
4:J:184:ASP:OD1	4:J:204:ARG:NH2	2.34	0.56
2:C:143:ALA:HB1	2:C:165:LEU:HD21	1.88	0.56
4:E:99:SER:HB3	4:E:124:VAL:H	1.69	0.56
2:C:131:ASN:HB3	2:C:181:MET:HE3	1.88	0.55
2:H:99:HIS:ND1	6:H:302:GOL:O2	2.32	0.55
4:E:133:PRO:HD3	4:E:252:PRO:HB3	1.88	0.54
2:C:163:THR:HG22	2:C:176:LEU:H	1.72	0.54
4:J:20:THR:H	6:J:301:GOL:HO2	1.55	0.53
4:J:99:SER:HB3	4:J:124:VAL:H	1.72	0.53
4:J:8:PRO:HG2	4:J:11:LEU:HD21	1.91	0.53
4:J:211:PHE:O	4:J:217:ASN:ND2	2.35	0.52
1:F:70:LEU:HD13	2:H:27:TYR:HB2	1.92	0.52
4:E:89:MET:HE1	4:E:102:TYR:CD1	2.46	0.51
2:C:115:PRO:HB3	2:C:140:PHE:HB3	1.92	0.51
2:H:72:GLY:N	2:H:73:PRO:HD2	2.25	0.51
4:J:141:PRO:HD3	4:J:154:LEU:HG	1.94	0.50
3:I:181:MET:HG2	6:J:302:GOL:H31	1.94	0.49
2:H:105:LEU:HD13	2:H:109:LEU:HD12	1.95	0.49
2:C:139:ASP:HA	2:C:172:THR:HB	1.95	0.49
2:H:139:ASP:HA	2:H:172:THR:HB	1.95	0.49
2:C:72:GLY:N	2:C:73:PRO:HD2	2.27	0.48
1:A:53:ARG:HD3	3:D:111:GLU:HG3	1.95	0.48
3:I:132:GLN:NE2	8:I:402:HOH:O	2.47	0.48
2:H:115:PRO:HB3	2:H:140:PHE:HB3	1.95	0.48
2:H:151:ARG:O	2:H:153:ASP:N	2.47	0.48
3:D:91:LEU:HD11	3:D:102:TYR:CE2	2.49	0.48
4:J:131:VAL:O	4:J:249:ARG:NH2	2.45	0.48
4:E:138:VAL:HG23	4:E:259:ALA:HB3	1.95	0.48
2:C:152:ASN:ND2	2:C:187:ASP:OD1	2.47	0.47
4:E:218:HIS:HB3	4:E:262:TRP:CD2	2.48	0.47
1:A:9(A):GLY:O	2:C:30:LYS:HA	2.15	0.47
4:J:89:MET:HE1	4:J:102:TYR:CD1	2.50	0.47
4:J:141:PRO:HG3	4:J:152:ALA:HB1	1.96	0.47
2:C:28:GLN:HB2	2:C:49:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:HIS:HA	6:F:205:GOL:H2	1.97	0.46
3:D:43:ARG:HB3	3:D:53:ILE:HD11	1.97	0.46
1:A:39:LYS:HG2	1:A:60:LEU:HD11	1.97	0.46
1:F:119:ILE:N	6:F:204:GOL:H31	2.22	0.46
4:J:132:PHE:CD1	4:J:198:ARG:HD3	2.51	0.46
1:A:30:GLU:OE2	1:A:33:TYR:HB3	2.16	0.45
3:D:197:LYS:O	3:D:199:ASP:N	2.42	0.45
3:I:43:ARG:HB3	3:I:53:ILE:HD11	1.99	0.45
3:I:45:ILE:HG13	3:I:100:ALA:HB2	1.98	0.45
2:H:99:HIS:HD1	6:H:302:GOL:HO2	1.57	0.45
3:D:47:SER:HB2	4:E:121:TRP:CZ2	2.51	0.45
1:A:178:TRP:CZ2	1:A:180:PRO:HA	2.52	0.44
1:A:43:TRP:CE3	1:A:48:PHE:HB3	2.52	0.44
4:J:6:GLN:NE2	4:J:102:TYR:O	2.49	0.44
6:I:301:GOL:H2	8:I:407:HOH:O	2.16	0.44
1:F:94:LYS:NZ	8:F:304:HOH:O	2.50	0.44
3:D:45:ILE:HG13	3:D:100:ALA:HB2	1.99	0.44
1:F:84:ASN:HA	1:F:114:PRO:HD3	2.00	0.43
2:C:152:ASN:HD21	2:C:187:ASP:HA	1.83	0.43
1:F:57:GLN:OE1	4:J:66:ARG:HD2	2.18	0.43
4:E:141:PRO:HD3	4:E:154:LEU:HG	2.01	0.43
2:C:133:LEU:HG	2:C:181:MET:HE2	2.01	0.43
2:H:9:GLU:HG3	2:H:10:VAL:H	1.83	0.43
4:E:101:LEU:HD13	4:E:121:TRP:CE2	2.53	0.43
3:D:47:SER:HB2	4:E:121:TRP:HZ2	1.83	0.43
2:H:102:GLN:O	2:H:106:ARG:HG2	2.19	0.42
4:E:44:GLN:HB2	4:E:50:LEU:HD13	2.00	0.42
1:F:39:LYS:HG2	1:F:60:LEU:HD11	2.00	0.42
2:C:163:THR:HG23	2:C:164:PRO:O	2.20	0.42
4:E:141:PRO:HG3	4:E:152:ALA:HB1	2.01	0.42
1:A:105:LEU:HD13	1:A:153:PHE:CE1	2.55	0.42
1:F:105:LEU:HD12	1:F:105:LEU:HA	1.89	0.42
4:E:5:THR:HB	4:E:24:SER:HB2	2.02	0.42
1:F:66:LEU:HG	2:H:27:TYR:CD1	2.54	0.41
4:J:45:THR:HG22	4:J:100:ALA:HB2	2.01	0.41
3:D:178:VAL:HG22	3:D:189:ASN:OD1	2.20	0.41
2:C:100:ASN:O	2:C:104:GLU:HG2	2.21	0.41
3:D:19:ALA:HB3	3:D:91:LEU:HB2	2.02	0.41
8:A:305:HOH:O	2:C:32:MET:HE3	2.19	0.41
2:C:88:ARG:NH2	8:C:406:HOH:O	2.54	0.41
1:F:105:LEU:HD11	1:F:178:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:GLU:HG3	2:C:10:VAL:H	1.86	0.41
2:H:45:VAL:HA	2:H:58:PHE:O	2.21	0.41
2:C:87:GLU:OE1	8:C:401:HOH:O	2.22	0.41
4:E:127:ASP:OD2	4:E:129:ASN:HB3	2.21	0.41
2:H:72:GLY:N	2:H:73:PRO:CD	2.84	0.41
2:H:143:ALA:HB2	2:H:173:PHE:CE1	2.56	0.41
3:D:161:THR:O	3:D:176:LYS:HD3	2.21	0.40
6:F:204:GOL:O3	6:F:204:GOL:O1	2.29	0.40
4:E:89:MET:HE1	4:E:102:TYR:CE1	2.56	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	181/185 (98%)	176 (97%)	5 (3%)	0	100	100
1	F	178/185 (96%)	175 (98%)	3 (2%)	0	100	100
2	C	188/213 (88%)	182 (97%)	6 (3%)	0	100	100
2	H	189/213 (89%)	181 (96%)	7 (4%)	1 (0%)	24	37
3	D	200/206 (97%)	189 (94%)	10 (5%)	1 (0%)	24	37
3	I	197/206 (96%)	189 (96%)	8 (4%)	0	100	100
4	E	238/240 (99%)	229 (96%)	9 (4%)	0	100	100
4	J	238/240 (99%)	231 (97%)	7 (3%)	0	100	100
All	All	1609/1688 (95%)	1552 (96%)	55 (3%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	152	ASN

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Mol	Chain	Res	Type
3	D	93	HIS

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	164/170 (96%)	163 (99%)	1 (1%)	78	89
1	F	159/170 (94%)	159 (100%)	0	100	100
2	C	159/189 (84%)	159 (100%)	0	100	100
2	H	154/189 (82%)	153 (99%)	1 (1%)	78	89
3	D	166/185 (90%)	166 (100%)	0	100	100
3	I	157/185 (85%)	156 (99%)	1 (1%)	78	89
4	E	205/210 (98%)	201 (98%)	4 (2%)	48	70
4	J	205/210 (98%)	202 (98%)	3 (2%)	57	77
All	All	1369/1508 (91%)	1359 (99%)	10 (1%)	76	88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
2	H	105	LEU
4	E	54	PHE
4	E	157	LEU
4	E	166	VAL
4	E	216	ARG
3	I	110	ILE
4	J	54	PHE
4	J	114	ILE
4	J	166	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	84	ASN
1	A	111	ASN
2	C	144	GLN
1	F	62	ASN
1	F	111	ASN
2	H	174	GLN
3	D	204	ASN
4	E	218	HIS
3	I	44	GLN
4	J	44	GLN
4	J	90	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](#)

23 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	$\# Z > 2$
7	PO4	I	303	-	4,4,4	0.94	0	6,6,6	0.48	0
6	GOL	I	302	-	5,5,5	0.86	0	5,5,5	1.04	0
6	GOL	F	205	-	5,5,5	0.96	0	5,5,5	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	J	302	-	5,5,5	0.88	0	5,5,5	1.07	0
6	GOL	F	203	-	5,5,5	0.93	0	5,5,5	1.06	0
6	GOL	E	301	-	5,5,5	0.98	0	5,5,5	1.03	0
6	GOL	J	301	-	5,5,5	0.90	0	5,5,5	1.10	0
7	PO4	E	302	-	4,4,4	0.91	0	6,6,6	0.51	0
7	PO4	A	205	-	4,4,4	0.93	0	6,6,6	0.45	0
5	NAG	F	202	-	14,14,15	0.24	0	17,19,21	0.42	0
5	NAG	H	301	2	14,14,15	0.29	0	17,19,21	0.40	0
5	NAG	A	201	1	14,14,15	0.37	0	17,19,21	0.50	0
7	PO4	D	302	-	4,4,4	0.93	0	6,6,6	0.45	0
5	NAG	F	201	1	14,14,15	0.25	0	17,19,21	0.47	0
6	GOL	D	301	-	5,5,5	0.89	0	5,5,5	1.12	0
6	GOL	A	203	-	5,5,5	0.92	0	5,5,5	1.07	0
6	GOL	F	204	-	5,5,5	0.98	0	5,5,5	0.98	0
7	PO4	C	301	-	4,4,4	0.92	0	6,6,6	0.44	0
6	GOL	I	301	-	5,5,5	0.96	0	5,5,5	1.06	0
7	PO4	J	303	-	4,4,4	0.93	0	6,6,6	0.46	0
6	GOL	H	302	-	5,5,5	0.88	0	5,5,5	1.08	0
6	GOL	A	204	-	5,5,5	0.96	0	5,5,5	1.06	0
5	NAG	A	202	1	14,14,15	0.26	0	17,19,21	0.37	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
5	NAG	A	201	1	-	3/6/23/26	0/1/1/1
6	GOL	F	203	-	-	0/4/4/4	-
6	GOL	E	301	-	-	1/4/4/4	-
6	GOL	I	301	-	-	2/4/4/4	-
5	NAG	F	201	1	-	2/6/23/26	0/1/1/1
6	GOL	D	301	-	-	1/4/4/4	-
6	GOL	H	302	-	-	1/4/4/4	-
6	GOL	J	301	-	-	4/4/4/4	-
6	GOL	A	203	-	-	0/4/4/4	-
5	NAG	A	202	1	-	2/6/23/26	0/1/1/1
6	GOL	A	204	-	-	0/4/4/4	-
5	NAG	F	202	-	-	4/6/23/26	0/1/1/1
6	GOL	F	204	-	-	0/4/4/4	-
6	GOL	I	302	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	F	205	-	-	2/4/4/4	-
5	NAG	H	301	2	-	2/6/23/26	0/1/1/1
6	GOL	J	302	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	301	GOL	O1-C1-C2-O2
6	J	301	GOL	O1-C1-C2-C3
5	F	202	NAG	O5-C5-C6-O6
5	A	201	NAG	O5-C5-C6-O6
5	A	201	NAG	C4-C5-C6-O6
5	F	202	NAG	C4-C5-C6-O6
5	F	202	NAG	C8-C7-N2-C2
5	F	202	NAG	O7-C7-N2-C2
5	H	301	NAG	C8-C7-N2-C2
5	H	301	NAG	O7-C7-N2-C2
5	F	201	NAG	O5-C5-C6-O6
5	F	201	NAG	C4-C5-C6-O6
5	A	202	NAG	O5-C5-C6-O6
6	F	205	GOL	C1-C2-C3-O3
6	D	301	GOL	O1-C1-C2-C3
6	E	301	GOL	O1-C1-C2-C3
6	I	302	GOL	O1-C1-C2-C3
6	J	301	GOL	C1-C2-C3-O3
6	J	301	GOL	O2-C2-C3-O3
6	F	205	GOL	O2-C2-C3-O3
6	H	302	GOL	O2-C2-C3-O3
5	A	202	NAG	C4-C5-C6-O6
6	I	301	GOL	C1-C2-C3-O3
5	A	201	NAG	C1-C2-N2-C7
6	I	301	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	302	GOL	2	0
6	F	205	GOL	1	0
6	J	302	GOL	1	0
6	J	301	GOL	1	0
6	F	204	GOL	3	0
6	I	301	GOL	1	0
6	H	302	GOL	2	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	183/185 (98%)	-0.19	3 (1%) 70 66	29, 43, 65, 100	0
1	F	180/185 (97%)	0.15	8 (4%) 39 34	35, 53, 90, 112	0
2	C	194/213 (91%)	0.18	11 (5%) 29 25	29, 48, 101, 116	0
2	H	195/213 (91%)	0.29	18 (9%) 14 12	34, 53, 105, 133	0
3	D	202/206 (98%)	0.21	13 (6%) 25 22	33, 50, 92, 109	0
3	I	201/206 (97%)	0.27	18 (8%) 15 12	32, 49, 92, 114	0
4	E	240/240 (100%)	-0.19	4 (1%) 69 65	30, 43, 68, 117	0
4	J	240/240 (100%)	-0.00	4 (1%) 69 65	34, 49, 78, 103	0
All	All	1635/1688 (96%)	0.08	79 (4%) 35 32	29, 48, 94, 133	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	219	SER	5.8
2	C	13	GLY	5.3
3	I	219	SER	4.6
2	C	185	ARG	4.3
1	F	179	GLU	4.1
2	H	14	GLY	3.8
2	C	207	ARG	3.7
3	I	169	SER	3.7
4	J	266	ASP	3.6
1	A	181	GLU	3.5
2	H	207	ARG	3.5
1	F	160	ILE	3.5
3	I	168	ASP	3.5
3	I	147	SER	3.5
3	D	211	ILE	3.5
3	I	165	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	158	ASP	3.4
1	A	158	ASP	3.3
3	I	196	ASN	3.3
2	C	186	GLY	3.3
2	H	131	ASN	3.3
2	H	160	VAL	3.2
3	D	167	LYS	3.2
2	H	185	ARG	3.1
1	F	124	ASN	3.1
3	I	213	GLU	3.1
3	D	47	SER	3.1
2	H	186	GLY	3.0
2	H	188	VAL	3.0
2	C	21	SER	3.0
2	C	182	THR	3.0
3	D	169	SER	3.0
2	C	188	VAL	2.9
3	D	2	MET	2.9
2	H	121	PRO	2.9
3	I	47	SER	2.8
3	I	214	ASP	2.8
1	F	128	VAL	2.7
2	C	11	CYS	2.7
3	I	204	ASN	2.6
1	A	180	PRO	2.6
2	H	184	GLN	2.6
3	I	210	ILE	2.6
3	D	165	GLN	2.6
3	I	197	LYS	2.5
2	H	39	THR	2.5
3	D	198	SER	2.5
2	H	132	LEU	2.4
4	E	48	GLN	2.4
2	C	121	PRO	2.4
3	D	213	GLU	2.4
3	D	148	ASP	2.3
3	D	196	ASN	2.3
1	F	125	GLY	2.3
2	H	182	THR	2.2
3	D	146	SER	2.2
3	I	170	ASP	2.2
4	J	196	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	206	TRP	2.2
2	C	161	VAL	2.2
2	H	181	MET	2.2
3	I	211	ILE	2.2
1	F	171	ASP	2.2
4	J	246	THR	2.2
2	H	21	SER	2.2
2	H	153	ASP	2.2
3	D	158	ASP	2.2
3	I	207	ASN	2.1
2	H	157	THR	2.1
1	F	99	LEU	2.1
2	C	203	ILE	2.1
4	E	242	ASN	2.1
4	J	260	GLU	2.1
3	I	148	ASP	2.1
2	H	183	PRO	2.1
3	I	160	GLN	2.0
4	E	241	GLU	2.0
3	I	208	ASN	2.0
4	E	266	ASP	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($\text{\AA}^2$)	Q<0.9
5	NAG	A	202	14/15	0.46	0.20	80,89,94,96	0
5	NAG	F	202	14/15	0.53	0.17	104,109,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	H	301	14/15	0.57	0.20	78,87,97,97	0
6	GOL	F	204	6/6	0.69	0.17	71,79,86,93	0
6	GOL	E	301	6/6	0.69	0.17	74,81,88,89	0
5	NAG	A	201	14/15	0.73	0.19	59,75,86,96	0
6	GOL	F	205	6/6	0.76	0.16	68,75,80,87	0
5	NAG	F	201	14/15	0.80	0.15	70,79,93,98	0
6	GOL	I	301	6/6	0.80	0.21	49,60,66,67	0
6	GOL	H	302	6/6	0.81	0.20	50,57,57,62	0
6	GOL	J	301	6/6	0.81	0.16	65,72,78,78	0
6	GOL	D	301	6/6	0.82	0.21	57,58,63,65	0
6	GOL	J	302	6/6	0.83	0.17	49,58,66,72	0
6	GOL	I	302	6/6	0.84	0.18	51,57,63,65	0
6	GOL	F	203	6/6	0.85	0.20	62,70,79,80	0
6	GOL	A	203	6/6	0.85	0.15	63,70,73,73	0
7	PO4	I	303	5/5	0.87	0.17	60,64,82,86	0
7	PO4	C	301	5/5	0.89	0.19	53,63,77,77	0
6	GOL	A	204	6/6	0.89	0.15	58,62,62,69	0
7	PO4	E	302	5/5	0.90	0.20	62,73,81,86	0
7	PO4	D	302	5/5	0.94	0.09	52,60,76,78	0
7	PO4	J	303	5/5	0.96	0.12	56,69,75,75	0
7	PO4	A	205	5/5	0.98	0.06	46,52,55,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.