



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:36 AM GMT

PDB ID : 2XN9  
Title : CRYSTAL STRUCTURE OF THE TERNARY COMPLEX BETWEEN HUMAN T CELL RECEPTOR, STAPHYLOCOCCAL ENTEROTOXIN H AND HUMAN MAJOR HISTOCOMPATIBILITY COMPLEX CLASS II  
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Deposited on : 2010-07-31  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

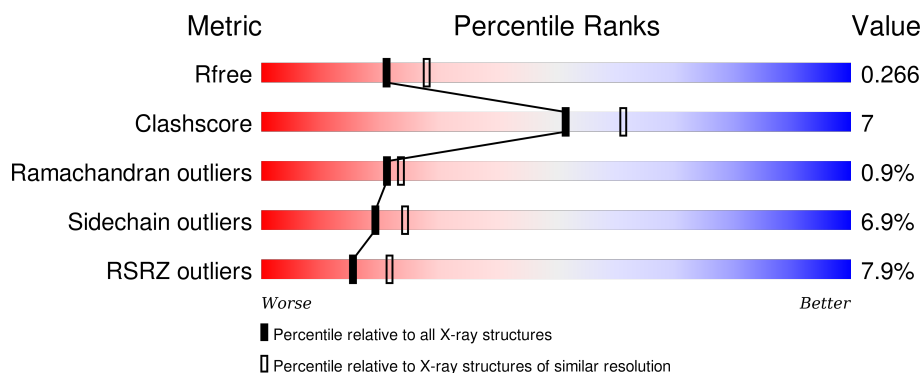
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	204	<div> <div>3%</div> <div>79%</div> <div>16%</div> <div>..</div> </div>
2	B	244	<div> <div>4%</div> <div>82%</div> <div>14%</div> <div>...</div> </div>
3	C	217	<div> <div>2%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
4	D	182	<div> <div>22%</div> <div>80%</div> <div>15%</div> <div>..</div> </div>
5	E	190	<div> <div>11%</div> <div>76%</div> <div>18%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	13	 <div>77%23%</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	B	1246	-	-	X	X
7	GOL	B	1247	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8711 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 T CELL RECEPTOR ALPHA CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	6	0
			1570	986	265	312	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	CYS	THR	ENGINEERED MUTATION	UNP P01848

- Molecule 2 is a protein called T CELL RECEPTOR BETA-1 CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	3	0
			1960	1234	339	381	6			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	118	LYS	ASN	CONFLICT	UNP P01850
B	119	ASN	LYS	CONFLICT	UNP P01850
B	151	TYR	PHE	CONFLICT	UNP P01850
B	171	CYS	SER	ENGINEERED MUTATION	UNP P01850
B	189	SER	CYS	CONFLICT	UNP P01850

- Molecule 3 is a protein called ENTEROTOXIN H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	215	Total	C	N	O	S	0	1	0
			1757	1108	287	359	3			

- Molecule 4 is a protein called HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN,.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	3	0
			1480	956	241	278	5			

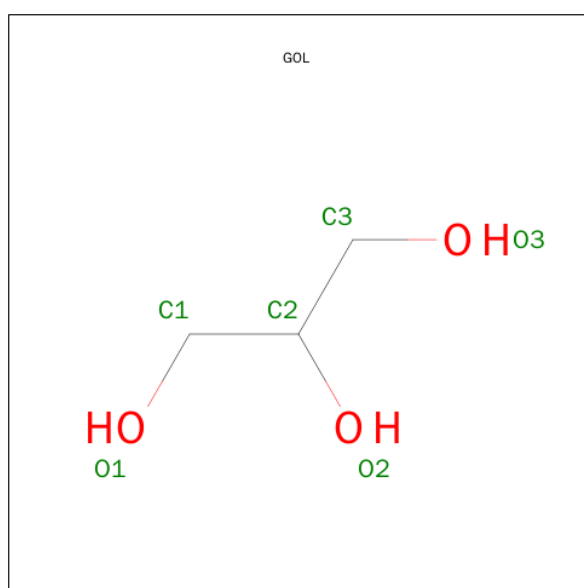
- Molecule 5 is a protein called MAJOR HISTOCOMPATIBILITY COMPLEX CLASS II BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	188	Total	C	N	O	S	0	2	0
			1534	963	274	291	6			

- Molecule 6 is a protein called HEMAGGLUTININ.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	13	Total	C	N	O	0	0	0
			105	69	18	18			

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Na	0	0
			1	1		

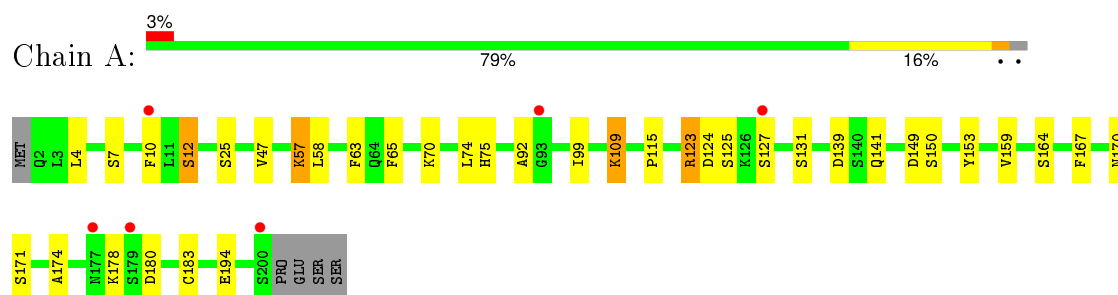
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	92	Total	O	0	0
			92	92		
9	B	74	Total	O	0	0
			74	74		
9	C	67	Total	O	0	0
			67	67		
9	D	25	Total	O	0	0
			25	25		
9	E	17	Total	O	0	0
			17	17		
9	F	5	Total	O	0	0
			5	5		

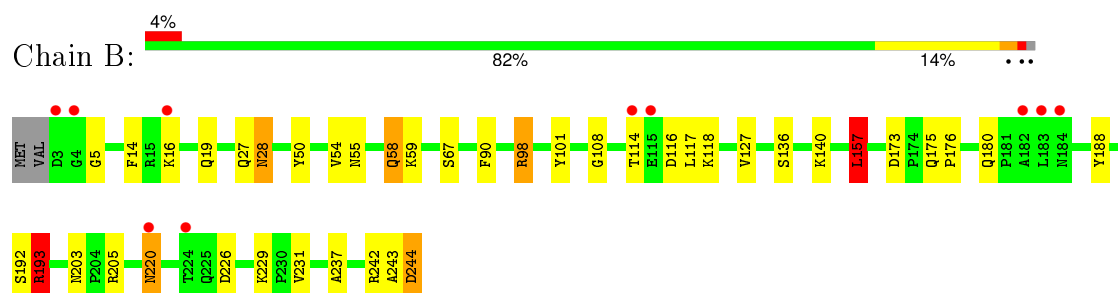
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

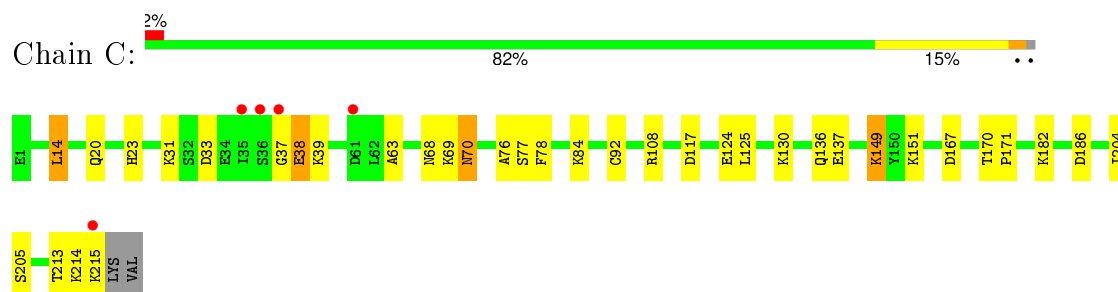
- Molecule 1: T CELL RECEPTOR ALPHA CHAIN C REGION



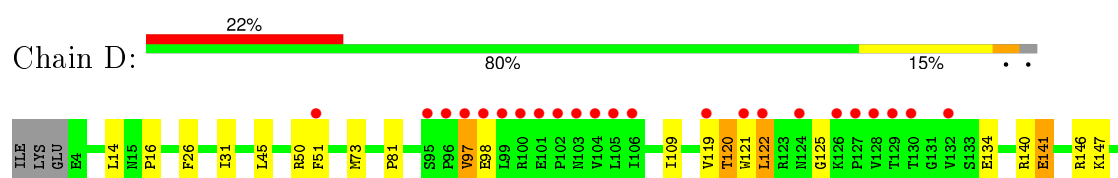
- Molecule 2: T CELL RECEPTOR BETA-1 CHAIN C REGION

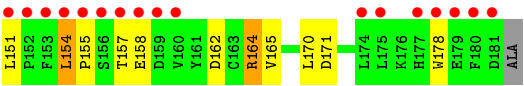


- Molecule 3: ENTEROTOXIN H

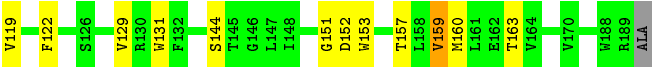


- Molecule 4: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN,

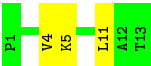




● Molecule 5: MAJOR HISTOCOMPATIBILITY COMPLEX CLASS II BETA CHAIN



● Molecule 6: HEMAGGLUTININ





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.18Å 48.89Å 166.72Å 90.00° 113.55° 90.00°	Depositor
Resolution (Å)	152.50 – 2.30 42.16 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (152.50-2.30) 97.2 (42.16-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.222 , 0.272 0.217 , 0.266	Depositor DCC
$R_{free}$ test set	3148 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.8	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 61849 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8711	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	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.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.78	1/1601 (0.1%)	0.76	0/2167
2	B	0.67	0/2013	0.75	3/2739 (0.1%)
3	C	0.63	0/1784	0.70	1/2399 (0.0%)
4	D	0.56	0/1525	0.64	0/2081
5	E	0.56	0/1573	0.71	0/2141
6	F	0.50	0/106	0.73	0/141
All	All	0.65	1/8602 (0.0%)	0.72	4/11668 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	CYS	CB-SG	5.35	1.91	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	193	ARG	NE-CZ-NH2	-7.39	116.60	120.30
2	B	157	LEU	CA-CB-CG	7.16	131.77	115.30
2	B	193	ARG	NE-CZ-NH1	5.97	123.28	120.30
3	C	14	LEU	CA-CB-CG	5.29	127.47	115.30

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	1570	0	1508	19	0
2	B	1960	0	1834	24	0
3	C	1757	0	1712	22	0
4	D	1480	0	1394	20	0
5	E	1534	0	1428	33	0
6	F	105	0	121	2	0
7	A	6	0	8	1	0
7	B	18	0	24	5	0
8	C	1	0	0	0	0
9	A	92	0	0	1	0
9	B	74	0	0	0	0
9	C	67	0	0	1	0
9	D	25	0	0	0	0
9	E	17	0	0	0	0
9	F	5	0	0	0	0
All	All	8711	0	8029	112	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 (112) 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:194[B]:GLU:H	1:A:194[B]:GLU:CD	1.56	0.97
5:E:129:VAL:HG11	5:E:159:VAL:HG21	1.57	0.86
5:E:23[B]:ARG:HH11	5:E:23[B]:ARG:HG3	1.43	0.83
3:C:213:THR:HG22	3:C:215:LYS:H	1.45	0.82
2:B:203:ASN:HD21	2:B:205:ARG:HH21	1.31	0.79
5:E:23[B]:ARG:HH11	5:E:23[B]:ARG:CG	1.98	0.75
1:A:171:SER:OG	2:B:193:ARG:HD3	1.89	0.72
5:E:129:VAL:CG1	5:E:159:VAL:HG21	2.19	0.71
5:E:117:CYS:HB3	5:E:159:VAL:HG23	1.75	0.69
5:E:129:VAL:HG11	5:E:159:VAL:CG2	2.23	0.68
5:E:81:HIS:CD2	6:F:4:VAL:HG23	2.28	0.67
1:A:194[B]:GLU:N	1:A:194[B]:GLU:CD	2.38	0.66
4:D:141[A]:GLU:OE2	4:D:141[A]:GLU:O	2.14	0.64
5:E:151:GLY:O	5:E:153:TRP:N	2.29	0.64
1:A:159:VAL:HG22	1:A:170:ASN:OD1	1.98	0.63
3:C:76:ALA:H	3:C:136:GLN:NE2	1.98	0.61
2:B:229:LYS:HG3	2:B:231:VAL:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:2:ASP:OD2	5:E:4:ARG:HD3	2.01	0.61
2:B:173:ASP:OD1	2:B:193:ARG:NH2	2.29	0.61
3:C:124:GLU:OE2	3:C:149:LYS:HE2	2.01	0.61
3:C:170:THR:HB	3:C:171:PRO:CD	2.32	0.60
4:D:120:THR:HB	4:D:164:ARG:HG2	1.85	0.58
2:B:50:TYR:CZ	2:B:58:GLN:HG3	2.39	0.58
2:B:188:TYR:HE1	7:B:1246:GOL:H31	1.68	0.58
4:D:140:ARG:HG2	4:D:146:ARG:HD2	1.86	0.57
4:D:81:PRO:HB3	5:E:5:PRO:HB2	1.86	0.57
4:D:134:GLU:OE2	4:D:147:LYS:NZ	2.37	0.57
3:C:213:THR:HG23	9:C:2067:HOH:O	2.05	0.56
1:A:194[B]:GLU:OE2	1:A:194[B]:GLU:N	2.38	0.55
2:B:28:ASN:HD22	2:B:28:ASN:H	1.53	0.55
1:A:123[B]:ARG:HD2	1:A:124:ASP:O	2.06	0.55
5:E:2:ASP:CG	5:E:6:ARG:HH22	2.10	0.55
5:E:23[B]:ARG:NH1	5:E:23[B]:ARG:CG	2.62	0.54
3:C:130:LYS:HE2	3:C:137:GLU:OE1	2.07	0.54
2:B:5:GLY:H	2:B:28:ASN:ND2	2.06	0.54
5:E:119:VAL:CG2	5:E:157:THR:HG22	2.39	0.53
3:C:37:GLY:O	3:C:38:GLU:HG2	2.09	0.53
5:E:97:PRO:HB3	5:E:122:PHE:HB3	1.91	0.52
2:B:98:ARG:HD2	2:B:98:ARG:H	1.74	0.52
1:A:149:ASP:C	1:A:149:ASP:OD1	2.48	0.52
1:A:57:LYS:O	1:A:58:LEU:HD13	2.08	0.52
1:A:74[B]:LEU:HD22	1:A:75:HIS:N	2.25	0.51
3:C:167:ASP:O	3:C:205:SER:HB3	2.10	0.51
2:B:188:TYR:CE1	7:B:1246:GOL:H31	2.47	0.49
3:C:170:THR:HB	3:C:171:PRO:HD2	1.95	0.49
2:B:14:PHE:CZ	2:B:114:THR:HB	2.48	0.49
5:E:2:ASP:OD2	5:E:6:ARG:NH2	2.45	0.49
4:D:122:LEU:HB2	4:D:162:ASP:HB2	1.94	0.49
3:C:117:ASP:OD2	3:C:213:THR:HB	2.13	0.49
5:E:2:ASP:O	5:E:3:THR:HG22	2.12	0.49
4:D:109:ILE:HD11	4:D:119:VAL:HG21	1.94	0.49
5:E:29:ARG:HH12	5:E:39:ARG:NH1	2.11	0.48
3:C:108:ARG:NH2	3:C:204:ILE:O	2.42	0.48
3:C:39:LYS:O	3:C:63:ALA:HB2	2.13	0.48
4:D:73:MET:HG2	6:F:11:LEU:CD1	2.44	0.48
2:B:127:VAL:HG23	2:B:237:ALA:HB3	1.96	0.47
5:E:108:PRO:HA	5:E:109:LEU:HA	1.77	0.47
4:D:26:PHE:HB2	4:D:31:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:GLY:H	2:B:28:ASN:HD21	1.62	0.47
2:B:243:ALA:N	2:B:244:ASP:HA	2.30	0.47
3:C:213:THR:HG22	3:C:214:LYS:N	2.30	0.46
3:C:77:SER:HA	3:C:92:CYS:O	2.15	0.46
5:E:74:ALA:HA	5:E:77:THR:OG1	2.16	0.46
4:D:51:PHE:CD2	4:D:51:PHE:N	2.83	0.46
5:E:74:ALA:O	5:E:78:TYR:HB3	2.15	0.46
2:B:176:PRO:HG2	7:B:1246:GOL:H32	1.97	0.46
2:B:14:PHE:CE1	2:B:114:THR:HB	2.51	0.46
2:B:101:TYR:HH	3:C:23:HIS:CE1	2.34	0.46
3:C:20:GLN:HE21	3:C:76:ALA:HB1	1.81	0.46
2:B:175:GLN:NE2	7:B:1246:GOL:O2	2.49	0.46
4:D:14:LEU:HD11	5:E:6:ARG:HB3	1.98	0.45
5:E:19:ASN:ND2	5:E:22:GLU:OE1	2.49	0.45
5:E:144:SER:HB2	5:E:159:VAL:HG12	1.97	0.45
1:A:167:PHE:CD2	2:B:140:LYS:HE2	2.53	0.44
7:A:1201:GOL:O3	7:B:1245:GOL:H12	2.17	0.44
5:E:117:CYS:HB2	5:E:131:TRP:CZ2	2.53	0.44
1:A:12:SER:OG	1:A:109[B]:LYS:HE2	2.18	0.44
1:A:153:TYR:O	1:A:174:ALA:HA	2.17	0.44
3:C:213:THR:CG2	3:C:214:LYS:N	2.80	0.43
1:A:109[A]:LYS:HB2	1:A:109[A]:LYS:HE3	1.42	0.43
5:E:113:ASN:HB3	5:E:163:THR:OG1	2.19	0.43
4:D:16:PRO:HD2	5:E:6:ARG:HD3	2.00	0.43
2:B:28:ASN:HD22	2:B:28:ASN:N	2.15	0.43
5:E:65:LYS:O	5:E:69:GLU:HG3	2.18	0.43
1:A:10[B]:PHE:C	1:A:10[B]:PHE:CD1	2.92	0.43
3:C:39:LYS:HB2	3:C:39:LYS:HE3	1.81	0.43
4:D:97:VAL:HG21	4:D:178:TRP:HZ2	1.84	0.43
3:C:182:LYS:HD3	3:C:182:LYS:HA	1.86	0.42
3:C:33:ASP:OD1	3:C:68:ASN:HB2	2.19	0.42
4:D:119:VAL:HG22	4:D:165:VAL:HG22	2.01	0.42
2:B:54:VAL:O	2:B:55:ASN:HB2	2.20	0.42
1:A:4:LEU:HD23	1:A:25:SER:HB2	2.01	0.42
3:C:78:PHE:HB3	3:C:186:ASP:HB3	2.02	0.42
1:A:178:LYS:HE2	1:A:180:ASP:HB3	2.02	0.42
4:D:109:ILE:CD1	4:D:119:VAL:HG21	2.51	0.41
4:D:154:LEU:HA	4:D:155:PRO:HD3	1.89	0.41
4:D:51:PHE:HD2	4:D:51:PHE:N	2.18	0.41
4:D:140:ARG:CG	4:D:146:ARG:HD2	2.50	0.41
2:B:16:LYS:HE3	2:B:117:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASP:OD2	1:A:139:ASP:C	2.59	0.41
5:E:18:PHE:HB2	5:E:23[B]:ARG:HB3	2.02	0.41
2:B:90:PHE:CZ	2:B:108:GLY:HA3	2.56	0.41
5:E:40:PHE:HB2	5:E:47:TYR:CE2	2.56	0.41
4:D:121:TRP:CE2	4:D:151:LEU:HB2	2.56	0.41
2:B:157:LEU:HD11	2:B:192:SER:CB	2.51	0.41
5:E:18:PHE:HB2	5:E:23[A]:ARG:HB3	2.03	0.40
1:A:92:ALA:O	9:A:2050:HOH:O	2.22	0.40
3:C:31:LYS:HD3	3:C:70:ASN:HD22	1.87	0.40
1:A:47:VAL:HG11	1:A:63:PHE:CG	2.56	0.40
5:E:119:VAL:HG23	5:E:119:VAL:O	2.22	0.40
4:D:73:MET:HG3	5:E:9:TRP:CZ3	2.57	0.40
5:E:21:THR:O	5:E:21:THR:HG23	2.22	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	203/204 (100%)	193 (95%)	9 (4%)	1 (0%)	34	41
2	B	243/244 (100%)	231 (95%)	9 (4%)	3 (1%)	16	16
3	C	214/217 (99%)	203 (95%)	10 (5%)	1 (0%)	34	41
4	D	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	30	36
5	E	188/190 (99%)	173 (92%)	11 (6%)	4 (2%)	9	7
6	F	11/13 (85%)	11 (100%)	0	0	100	100
All	All	1038/1050 (99%)	979 (94%)	49 (5%)	10 (1%)	21	21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	152	ASP
3	C	38	GLU
2	B	226[A]	ASP
2	B	226[B]	ASP
4	D	125	GLY
1	A	127	SER
2	B	220	ASN
5	E	3	THR
5	E	106	THR
5	E	107	GLN

### 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	176/180 (98%)	160 (91%)	16 (9%)	12	13
2	B	212/215 (99%)	196 (92%)	16 (8%)	17	21
3	C	194/197 (98%)	187 (96%)	7 (4%)	42	57
4	D	163/166 (98%)	149 (91%)	14 (9%)	13	15
5	E	165/171 (96%)	153 (93%)	12 (7%)	17	22
6	F	12/12 (100%)	11 (92%)	1 (8%)	14	17
All	All	922/941 (98%)	856 (93%)	66 (7%)	19	22

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	12	SER
1	A	57	LYS
1	A	65	PHE
1	A	70	LYS
1	A	99	ILE
1	A	109[A]	LYS
1	A	109[B]	LYS
1	A	115	PRO

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Mol	Chain	Res	Type
1	A	123[A]	ARG
1	A	123[B]	ARG
1	A	125	SER
1	A	131	SER
1	A	141	GLN
1	A	150	SER
1	A	164	SER
2	B	19	GLN
2	B	27	GLN
2	B	28	ASN
2	B	58	GLN
2	B	59	LYS
2	B	67	SER
2	B	98	ARG
2	B	116	ASP
2	B	118	LYS
2	B	136	SER
2	B	157	LEU
2	B	180	GLN
2	B	193	ARG
2	B	220	ASN
2	B	242	ARG
2	B	244	ASP
3	C	14	LEU
3	C	69	LYS
3	C	70	ASN
3	C	84	LYS
3	C	125	LEU
3	C	149	LYS
3	C	151	LYS
4	D	45	LEU
4	D	50	ARG
4	D	97	VAL
4	D	98	GLU
4	D	120	THR
4	D	122	LEU
4	D	141[A]	GLU
4	D	141[B]	GLU
4	D	154	LEU
4	D	157	THR
4	D	158	GLU
4	D	164	ARG

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Mol	Chain	Res	Type
4	D	170	LEU
4	D	171	ASP
5	E	3	THR
5	E	6	ARG
5	E	21	THR
5	E	39	ARG
5	E	50	VAL
5	E	65	LYS
5	E	67	LEU
5	E	94	ARG
5	E	107	GLN
5	E	113	ASN
5	E	159	VAL
5	E	160	MET
6	F	5	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	27	GLN
2	B	28	ASN
2	B	167	HIS
2	B	175	GLN
2	B	184	ASN
2	B	233	GLN
3	C	20	GLN
3	C	29	ASN
3	C	70	ASN
3	C	136	GLN
4	D	149	HIS
5	E	113	ASN
6	F	6	GLN
6	F	7	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	GOL	A	1201	-	5,5,5	0.48	0	5,5,5	0.47	0
7	GOL	B	1245	-	5,5,5	0.43	0	5,5,5	0.57	0
7	GOL	B	1246	-	5,5,5	0.37	0	5,5,5	0.25	0
7	GOL	B	1247	-	5,5,5	0.35	0	5,5,5	0.24	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	GOL	A	1201	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1245	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1246	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1247	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1201	GOL	1	0
7	B	1245	GOL	1	0
7	B	1246	GOL	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	199/204 (97%)	0.26	6 (3%) 54 63	12, 24, 46, 55	0
2	B	242/244 (99%)	0.25	10 (4%) 41 50	10, 32, 53, 67	0
3	C	215/217 (99%)	0.07	5 (2%) 64 72	23, 37, 52, 60	0
4	D	178/182 (97%)	0.99	40 (22%) 1 1	29, 49, 81, 86	0
5	E	188/190 (98%)	0.64	21 (11%) 7 10	29, 50, 71, 86	0
6	F	13/13 (100%)	0.13	0 100 100	30, 34, 41, 43	0
All	All	1035/1050 (98%)	0.41	82 (7%) 15 22	10, 38, 71, 86	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	111	HIS	7.2
5	E	109	LEU	6.7
4	D	160	VAL	6.6
4	D	180	PHE	6.1
4	D	157	THR	5.5
4	D	129	THR	5.4
4	D	155	PRO	5.1
5	E	108	PRO	5.1
2	B	182	ALA	4.9
4	D	97	VAL	4.8
2	B	3	ASP	4.3
4	D	127	PRO	4.3
4	D	153	PHE	4.2
1	A	127	SER	4.2
4	D	156	SER	4.2
4	D	154	LEU	4.1
4	D	128	VAL	4.1
4	D	95	SER	4.0
4	D	158	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
4	D	96	PRO	3.6
4	D	105	LEU	3.6
4	D	181	ASP	3.6
3	C	35	ILE	3.4
5	E	105	LYS	3.4
4	D	98	GLU	3.3
4	D	178	TRP	3.2
5	E	170	VAL	3.2
2	B	115	GLU	3.2
4	D	121	TRP	3.2
4	D	151	LEU	3.2
5	E	106	THR	3.2
5	E	110	GLN	3.1
5	E	145	THR	3.1
5	E	146	GLY	3.1
2	B	4	GLY	3.1
4	D	51	PHE	3.1
4	D	179	GLU	3.0
2	B	183	LEU	3.0
1	A	93	GLY	2.9
3	C	61	ASP	2.9
1	A	200	SER	2.9
2	B	224	THR	2.9
4	D	152	PRO	2.9
5	E	102	TYR	2.8
4	D	130	THR	2.8
5	E	148	ILE	2.8
5	E	161	LEU	2.8
5	E	112	HIS	2.7
1	A	179	SER	2.7
4	D	102	PRO	2.7
4	D	106	ILE	2.7
4	D	99	LEU	2.7
4	D	159	ASP	2.7
4	D	177	HIS	2.7
5	E	132	PHE	2.7
4	D	122	LEU	2.6
4	D	124	ASN	2.6
1	A	177	ASN	2.6
4	D	126	LYS	2.5
4	D	119	VAL	2.5
2	B	114	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	215	LYS	2.4
4	D	103	ASN	2.3
5	E	58	ALA	2.3
5	E	164	VAL	2.3
2	B	184	ASN	2.3
4	D	132	VAL	2.2
4	D	175	LEU	2.2
4	D	100	ARG	2.2
5	E	126	SER	2.2
1	A	10[A]	PHE	2.1
3	C	36	SER	2.1
4	D	174	LEU	2.1
5	E	114	LEU	2.1
3	C	37	GLY	2.1
5	E	65	LYS	2.1
2	B	16	LYS	2.1
5	E	188	TRP	2.1
4	D	104	VAL	2.1
2	B	220	ASN	2.0
5	E	104	SER	2.0
4	D	101	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	B	1246	6/6	0.81	0.26	5.65	69,69,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	B	1247	6/6	0.76	0.27	2.47	77,78,79,79	0
7	GOL	A	1201	6/6	0.80	0.22	1.89	42,49,51,51	0
7	GOL	B	1245	6/6	0.87	0.18	1.61	34,38,40,40	0
8	NA	C	1216	1/1	0.99	0.09	-1.50	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.