



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:04 PM GMT

PDB ID : 4H25
Title : TCR interaction with peptide mimics of nickel offers structure insights to nickel contact allergy
Authors : Kappler, J.W.; Yin, L.; Dai, S.; Marrack, P.; Crawford, F.
Deposited on : 2012-09-12
Resolution : 2.20 Å(reported)

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

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

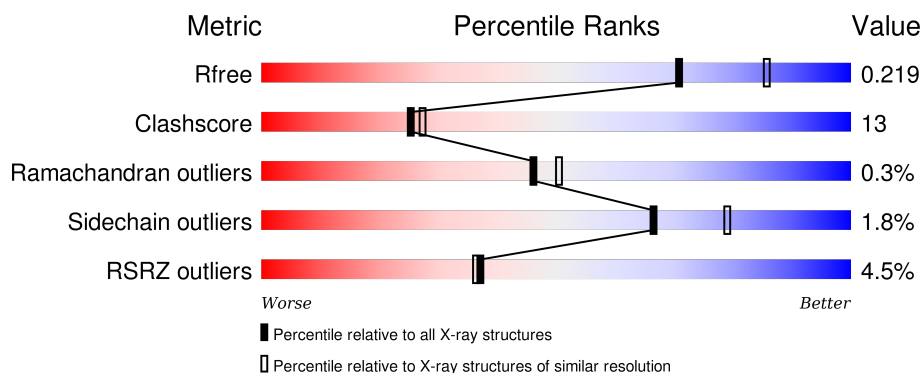
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	180	<div> <div>3%</div> <div>81%19%</div> </div>
1	D	180	<div> <div>8%</div> <div>81%19%</div> </div>
2	B	188	<div> <div>2%</div> <div>72%27%</div> </div>
2	E	188	<div> <div>5%</div> <div>72%24%</div> </div>
3	C	22	<div> <div>9%</div> <div>73%23%5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	22	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	IPA	A	205	-	-	-	X
5	IPA	E	203	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6910 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, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1479	957	240	277	5			
1	D	180	Total	C	N	O	S	0	0	0
			1479	957	240	277	5			

- Molecule 2 is a protein called MHC class II antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	S	0	0	0
			1549	978	279	287	5			
2	E	182	Total	C	N	O	S	0	0	0
			1496	945	267	279	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	THR	-	EXPRESSION TAG	UNP B8YAC7
B	4	ARG	-	EXPRESSION TAG	UNP B8YAC7
B	5	PRO	-	EXPRESSION TAG	UNP B8YAC7
B	77	THR	ASN	CONFLICT	UNP B8YAC7
B	189	ARG	-	EXPRESSION TAG	UNP B8YAC7
B	190	ALA	-	EXPRESSION TAG	UNP B8YAC7
E	3	THR	-	EXPRESSION TAG	UNP B8YAC7
E	4	ARG	-	EXPRESSION TAG	UNP B8YAC7
E	5	PRO	-	EXPRESSION TAG	UNP B8YAC7
E	77	THR	ASN	CONFLICT	UNP B8YAC7
E	189	ARG	-	EXPRESSION TAG	UNP B8YAC7
E	190	ALA	-	EXPRESSION TAG	UNP B8YAC7

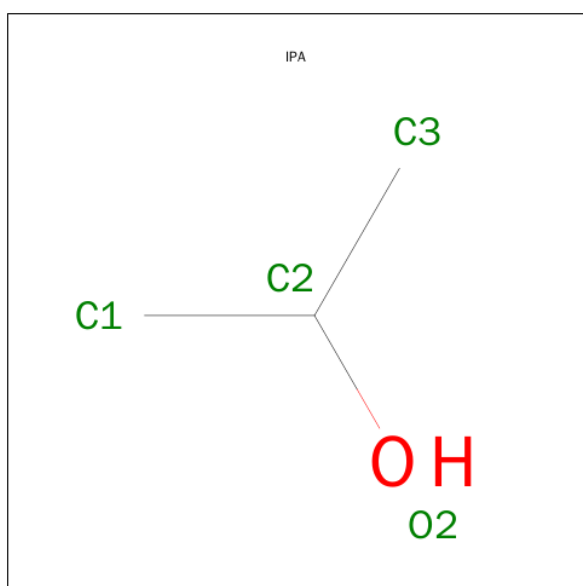
- Molecule 3 is a protein called peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	22	Total	C	N	O	S	0	0	0
			174	109	37	27	1			
3	F	22	Total	C	N	O	S	0	0	0
			174	109	37	27	1			

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	3	1		
5	A	1	Total	C	O	0	0
			4	3	1		

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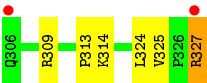
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	3	1		
5	E	1	Total	C	O	0	0
			4	3	1		

- Molecule 6 is water.

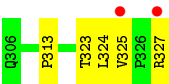
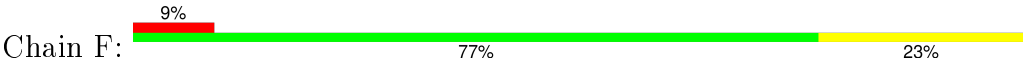
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	104	Total	O	0	0
			104	104		
6	B	114	Total	O	0	0
			114	114		
6	C	15	Total	O	0	0
			15	15		
6	D	63	Total	O	0	0
			63	63		
6	E	58	Total	O	0	0
			58	58		
6	F	21	Total	O	0	0
			21	21		



● Molecule 3: peptide



● Molecule 3: peptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.52Å 97.18Å 67.10Å 90.00° 105.36° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 47.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.20) 93.5 (47.42-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.255 0.214 , 0.219	Depositor DCC
R_{free} test set	2317 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 45484 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6910	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: IPA, NAG

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	0.40	0/1524	0.61	0/2077
1	D	0.36	0/1524	0.56	0/2077
2	B	0.43	0/1591	0.65	0/2160
2	E	0.37	0/1534	0.57	0/2080
3	C	0.31	0/177	0.59	0/237
3	F	0.36	0/177	0.62	0/237
All	All	0.38	0/6527	0.60	0/8868

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	1479	0	1410	29	0
1	D	1479	0	1410	34	0
2	B	1549	0	1479	51	0
2	E	1496	0	1430	48	0
3	C	174	0	193	12	0
3	F	174	0	193	5	0
4	A	56	0	50	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	28	0	25	0	0
4	D	56	0	50	5	0
4	E	28	0	25	1	0
5	A	8	0	16	2	0
5	B	4	0	8	1	0
5	E	4	0	8	1	0
6	A	104	0	0	3	0
6	B	114	0	0	4	0
6	C	15	0	0	1	0
6	D	63	0	0	2	0
6	E	58	0	0	4	0
6	F	21	0	0	1	0
All	All	6910	0	6297	161	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 13.

All (161) 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:D:87:PRO:HD2	1:D:170:LEU:HD11	1.44	0.98
1:D:167:HIS:HB3	1:D:170:LEU:HD13	1.62	0.81
2:E:55:ARG:HB2	2:E:56:PRO:HD3	1.64	0.78
3:C:327:ARG:HE	3:C:327:ARG:H	1.29	0.77
2:B:52:GLU:HG2	2:B:55:ARG:HH12	1.51	0.76
2:E:116:VAL:HG22	2:E:160:MET:HG2	1.69	0.74
2:B:105:LYS:HE2	2:B:111:HIS:HA	1.68	0.74
2:E:4:ARG:HG2	3:F:327:ARG:HG3	1.71	0.72
2:B:133:ARG:HH12	2:B:138:GLU:HG2	1.55	0.72
4:E:201:NAG:O3	4:E:202:NAG:H2	1.90	0.71
2:B:138:GLU:HG3	6:B:409:HOH:O	1.91	0.70
1:D:93:THR:HB	1:D:103:ASN:HD21	1.57	0.70
2:B:10:LEU:HB3	2:B:31:PHE:HB2	1.75	0.69
2:B:11:LEU:CD2	3:C:313:PRO:HB3	2.24	0.68
4:A:201:NAG:H2	4:A:202:NAG:O3	1.94	0.68
2:B:11:LEU:HD21	3:C:313:PRO:HB3	1.77	0.66
2:B:55:ARG:HB2	2:B:56:PRO:HD3	1.76	0.66
2:E:163:THR:O	2:E:165:PRO:HD3	1.96	0.66
2:B:107:GLN:HE21	2:B:110:GLN:HB2	1.61	0.65
1:A:16:PRO:HD2	2:B:6:ARG:HD3	1.77	0.65
1:A:168:TRP:CE2	4:A:204:NAG:H83	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:HD12	5:A:205:IPA:H2	1.79	0.63
2:B:105:LYS:HG3	2:B:112:HIS:HD2	1.63	0.62
3:F:327:ARG:HD3	6:F:401:HOH:O	2.01	0.60
1:D:118:ASN:HB2	1:D:166:GLU:HB2	1.84	0.60
1:A:11:GLU:OE1	1:A:62:ASN:HB3	2.01	0.60
1:D:87:PRO:HB3	1:D:112:PHE:HB3	1.82	0.60
2:E:3:THR:HG23	2:E:6:ARG:HH12	1.66	0.60
1:D:87:PRO:HD2	1:D:170:LEU:CD1	2.25	0.59
1:A:110:ASP:OD1	1:A:140:ARG:HD2	2.02	0.59
2:E:65:LYS:HE2	2:E:65:LYS:HA	1.85	0.58
1:A:111:LYS:HG2	1:A:140:ARG:CZ	2.33	0.58
1:A:147:LYS:HE3	1:A:149:HIS:CE1	2.41	0.56
1:D:70:LEU:HB2	2:E:9:GLU:HB2	1.89	0.55
2:B:94:ARG:HH11	2:B:94:ARG:HG3	1.71	0.55
3:C:327:ARG:HE	3:C:327:ARG:N	2.00	0.55
1:A:47:GLU:HG3	6:B:400:HOH:O	2.06	0.55
2:B:67:LEU:HD21	3:C:314:LYS:HG3	1.89	0.54
2:B:94:ARG:NH1	2:B:94:ARG:HG3	2.22	0.54
1:A:70:LEU:HB2	2:B:9:GLU:HB2	1.89	0.53
1:D:134:GLU:OE2	1:D:147:LYS:NZ	2.42	0.53
1:D:9:GLN:HB3	2:E:13:SER:HB2	1.91	0.53
2:B:36:GLU:HG2	2:B:50:VAL:HG21	1.90	0.52
2:B:105:LYS:HG3	2:B:112:HIS:CD2	2.45	0.52
4:D:603:NAG:O3	4:D:603:NAG:H83	2.09	0.52
2:B:7:PHE:CE2	3:C:325:VAL:HB	2.44	0.52
2:E:157:THR:C	2:E:158:LEU:HD12	2.31	0.51
2:E:11:LEU:CD2	3:F:313:PRO:HB3	2.39	0.51
2:E:11:LEU:HD22	3:F:313:PRO:HB3	1.92	0.51
2:E:172:THR:CG2	2:E:185:THR:HG23	2.41	0.51
2:B:52:GLU:HG2	2:B:55:ARG:NH1	2.23	0.51
1:D:26:PHE:HB2	1:D:31:ILE:HD11	1.93	0.51
1:A:36:MET:O	1:A:39:LYS:HD2	2.11	0.51
5:B:203:IPA:H12	3:C:309:ARG:HD3	1.93	0.51
1:D:105:LEU:HG	1:D:153:PHE:CE1	2.46	0.50
2:B:11:LEU:HD22	3:C:313:PRO:HB3	1.94	0.50
2:E:94:ARG:HH11	2:E:94:ARG:HG3	1.76	0.50
1:D:97:VAL:HA	6:D:705:HOH:O	2.11	0.50
2:B:74:GLN:HA	2:B:74:GLN:NE2	2.27	0.50
1:D:113:THR:HG21	2:E:34:GLN:HE21	1.77	0.50
5:A:205:IPA:H32	6:A:378:HOH:O	2.12	0.49
3:C:327:ARG:NE	3:C:327:ARG:H	2.06	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:PHE:C	2:B:27:LEU:HD12	2.32	0.49
1:A:11:GLU:O	2:B:10:LEU:HD12	2.13	0.49
2:B:83:TYR:O	2:B:87:GLU:HB2	2.13	0.49
1:A:162:ASP:HA	1:A:176:LYS:O	2.11	0.49
1:D:87:PRO:HB3	1:D:112:PHE:CB	2.43	0.49
1:D:113:THR:OG1	1:D:114:PRO:HA	2.13	0.48
2:E:3:THR:HG23	2:E:6:ARG:NH1	2.28	0.48
1:D:97:VAL:HG12	1:D:103:ASN:HD22	1.77	0.48
2:B:9:GLU:OE1	2:B:32:HIS:HD2	1.96	0.48
1:D:11:GLU:OE1	1:D:62:ASN:HB3	2.13	0.48
2:E:10:LEU:HD21	2:E:12:LYS:HE3	1.93	0.48
2:B:100:THR:HG22	3:F:323:THR:HG23	1.96	0.48
4:D:601:NAG:H83	4:D:602:NAG:H62	1.95	0.48
2:B:18:PHE:HB2	2:B:23:ARG:HB3	1.96	0.48
2:B:52:GLU:HA	2:B:55:ARG:NH1	2.29	0.48
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.96	0.48
2:E:3:THR:HG22	6:E:342:HOH:O	2.15	0.47
1:D:70:LEU:HD13	2:E:9:GLU:HB2	1.96	0.47
1:A:108:PHE:CZ	1:A:110:ASP:HB2	2.49	0.47
2:B:3:THR:HB	2:B:6:ARG:NH2	2.30	0.47
2:E:132:PHE:HB2	2:E:172:THR:HB	1.96	0.47
1:A:170:LEU:HD21	1:A:174:LEU:HB2	1.95	0.47
2:E:4:ARG:O	2:E:6:ARG:NH1	2.48	0.47
1:D:105:LEU:HG	1:D:153:PHE:CD1	2.50	0.47
2:E:25:ARG:NE	2:E:27:LEU:HD11	2.30	0.47
2:B:106:THR:HG22	2:B:114:LEU:HD22	1.97	0.46
2:B:164:VAL:HG13	6:B:404:HOH:O	2.16	0.46
2:E:117:CYS:HB2	2:E:131:TRP:CZ2	2.51	0.46
2:B:40:PHE:HB2	2:B:47:TYR:CE2	2.51	0.46
4:D:603:NAG:H82	4:D:604:NAG:H82	1.98	0.46
2:E:94:ARG:HG3	2:E:94:ARG:NH1	2.31	0.46
2:E:114:LEU:HD12	2:E:162:GLU:HA	1.97	0.46
1:D:11:GLU:O	2:E:10:LEU:HD12	2.16	0.46
2:E:26:PHE:C	2:E:27:LEU:HD12	2.36	0.46
2:B:48:ARG:HH11	2:B:48:ARG:HG3	1.80	0.46
1:D:16:PRO:HD2	2:E:6:ARG:HD2	1.97	0.46
1:A:116:VAL:HG12	4:A:204:NAG:H82	1.97	0.46
2:E:172:THR:HG23	2:E:185:THR:HG23	1.99	0.45
1:A:95:SER:HB2	1:A:96:PRO:CD	2.47	0.45
2:E:29:ARG:HB3	2:E:36:GLU:OE2	2.15	0.45
2:B:164:VAL:HA	6:B:404:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:96:HIS:HA	2:E:97:PRO:HD3	1.81	0.45
2:E:96:HIS:HD2	2:E:179:SER:HB2	1.81	0.45
2:B:129:VAL:HB	2:B:159:VAL:HG21	1.99	0.45
2:B:107:GLN:NE2	2:B:110:GLN:HB2	2.27	0.45
1:A:176:LYS:HD3	1:A:176:LYS:HA	1.83	0.45
4:D:601:NAG:C8	4:D:602:NAG:H62	2.47	0.44
2:E:38:VAL:HG22	2:E:39:ARG:N	2.32	0.44
1:D:92:LEU:HD23	1:D:92:LEU:N	2.32	0.44
2:B:107:GLN:O	2:B:107:GLN:HG3	2.17	0.44
1:A:110:ASP:OD1	1:A:140:ARG:NH1	2.50	0.44
2:B:67:LEU:CD2	3:C:314:LYS:HG3	2.48	0.44
2:B:10:LEU:HD21	2:B:12:LYS:HE3	1.99	0.44
2:E:31:PHE:CE2	2:E:36:GLU:HB2	2.53	0.44
2:B:67:LEU:HD22	3:C:314:LYS:HE3	2.00	0.44
2:B:132:PHE:HB2	2:B:172:THR:HB	1.99	0.44
2:B:110:GLN:HB3	2:B:111:HIS:H	1.66	0.43
2:E:74:GLN:HE22	5:E:203:IPA:H2	1.81	0.43
1:D:170:LEU:HD12	1:D:170:LEU:N	2.33	0.43
1:A:11:GLU:CD	2:B:11:LEU:HD23	2.39	0.43
1:D:123:ARG:HB2	1:D:128:VAL:HG21	2.00	0.43
2:E:36:GLU:OE2	2:E:39:ARG:HD2	2.19	0.43
2:B:97:PRO:HB3	2:B:122:PHE:HB3	2.01	0.43
6:D:713:HOH:O	2:E:120:SER:HB2	2.18	0.43
2:B:55:ARG:O	2:B:59:GLU:HG3	2.19	0.42
2:E:75:VAL:HG13	6:E:315:HOH:O	2.18	0.42
1:A:14:LEU:HD12	2:B:7:PHE:O	2.20	0.42
3:C:324:LEU:HB3	6:C:414:HOH:O	2.19	0.42
1:D:87:PRO:CB	1:D:112:PHE:HB3	2.49	0.42
2:B:74:GLN:HE21	2:B:74:GLN:HA	1.84	0.42
2:E:47:TYR:OH	2:E:71:LYS:HE3	2.20	0.42
1:D:124:ASN:HD21	1:D:159:ASP:HA	1.84	0.42
1:A:149:HIS:HD2	6:A:351:HOH:O	2.01	0.41
1:D:113:THR:OG1	2:E:34:GLN:NE2	2.53	0.41
1:A:80:THR:HA	1:A:81:PRO:HD3	1.92	0.41
1:A:147:LYS:HE3	1:A:149:HIS:HE1	1.83	0.41
6:A:342:HOH:O	2:B:32:HIS:HE1	2.03	0.41
1:A:122:LEU:HD23	1:A:127:PRO:HA	2.02	0.41
1:A:140:ARG:CG	1:A:146:ARG:HG3	2.51	0.41
2:B:114:LEU:HD12	2:B:162:GLU:HA	2.01	0.41
1:D:87:PRO:HB3	1:D:112:PHE:CG	2.56	0.41
1:D:29:ASP:HB3	2:E:153:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:PRO:HD2	2:E:6:ARG:CD	2.51	0.41
2:E:4:ARG:HD3	6:E:324:HOH:O	2.21	0.41
1:D:97:VAL:HG12	1:D:103:ASN:ND2	2.36	0.41
4:D:603:NAG:C1	4:D:604:NAG:HN2	2.34	0.41
2:E:74:GLN:HA	2:E:74:GLN:NE2	2.36	0.41
2:E:74:GLN:HA	2:E:74:GLN:HE21	1.85	0.41
1:A:97:VAL:HG11	1:A:178:TRP:HZ2	1.86	0.41
2:E:77:THR:O	2:E:77:THR:HG22	2.20	0.41
2:B:17:PHE:HB3	2:B:20:GLY:O	2.21	0.41
1:A:140:ARG:HG3	1:A:146:ARG:HG3	2.02	0.40
1:A:95:SER:HB2	1:A:96:PRO:HD2	2.03	0.40
1:D:99:LEU:C	1:D:101:GLU:H	2.25	0.40
2:B:145:THR:HB	2:B:148:ILE:HD11	2.03	0.40
1:D:97:VAL:HG11	1:D:178:TRP:CZ2	2.57	0.40
1:D:11:GLU:CD	2:E:11:LEU:HD23	2.41	0.40
2:E:40:PHE:HB2	2:E:47:TYR:CE2	2.57	0.40
2:E:180:VAL:HG23	6:E:322:HOH:O	2.21	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	178/180 (99%)	174 (98%)	4 (2%)	0	100	100
1	D	178/180 (99%)	170 (96%)	8 (4%)	0	100	100
2	B	186/188 (99%)	179 (96%)	5 (3%)	2 (1%)	17	14
2	E	178/188 (95%)	170 (96%)	8 (4%)	0	100	100
3	C	20/22 (91%)	20 (100%)	0	0	100	100
3	F	20/22 (91%)	20 (100%)	0	0	100	100
All	All	760/780 (97%)	733 (96%)	25 (3%)	2 (0%)	46	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	109	LEU
2	B	110	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	164/164 (100%)	162 (99%)	2 (1%)	78	88
1	D	164/164 (100%)	160 (98%)	4 (2%)	57	69
2	B	172/172 (100%)	170 (99%)	2 (1%)	78	88
2	E	166/172 (96%)	164 (99%)	2 (1%)	78	88
3	C	20/20 (100%)	19 (95%)	1 (5%)	30	35
3	F	20/20 (100%)	18 (90%)	2 (10%)	9	8
All	All	706/712 (99%)	693 (98%)	13 (2%)	66	79

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	VAL
1	A	181	ASP
2	B	34	GLN
2	B	35	GLU
3	C	327	ARG
1	D	130	THR
1	D	142	ASP
1	D	171	ASP
1	D	181	ASP
2	E	4	ARG
2	E	67	LEU
3	F	324	LEU
3	F	325	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	A	149	HIS
2	B	32	HIS
2	B	74	GLN
2	B	96	HIS
2	B	107	GLN
2	B	110	GLN
2	B	112	HIS
2	B	156	GLN
3	C	306	GLN
1	D	18	GLN
1	D	103	ASN
1	D	143	HIS
1	D	149	HIS
2	E	34	GLN
2	E	74	GLN
2	E	96	HIS
2	E	113	ASN
2	E	150	ASN

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 ⓘ

12 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	201	4	14,14,15	0.49	0	15,19,21	0.77	1 (6%)
4	NAG	A	202	1,4	14,14,15	0.58	0	15,19,21	0.77	1 (6%)
4	NAG	A	203	4	14,14,15	0.46	0	15,19,21	0.82	1 (6%)
4	NAG	A	204	1,4	14,14,15	0.55	0	15,19,21	0.76	1 (6%)
4	NAG	B	201	4	14,14,15	0.40	0	15,19,21	0.77	1 (6%)
4	NAG	B	202	2,4	14,14,15	0.54	0	15,19,21	0.83	1 (6%)
4	NAG	D	601	4	14,14,15	0.43	0	15,19,21	0.72	1 (6%)
4	NAG	D	602	1,4	14,14,15	0.44	0	15,19,21	0.69	0
4	NAG	D	603	4	14,14,15	0.50	0	15,19,21	0.71	1 (6%)
4	NAG	D	604	1,4	14,14,15	0.69	0	15,19,21	1.04	1 (6%)
4	NAG	E	201	2,4	14,14,15	0.60	0	15,19,21	0.82	1 (6%)
4	NAG	E	202	4	14,14,15	0.53	0	15,19,21	0.71	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	201	4	-	0/6/23/26	0/1/1/1
4	NAG	A	202	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	203	4	-	0/6/23/26	0/1/1/1
4	NAG	A	204	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	201	4	-	0/6/23/26	0/1/1/1
4	NAG	B	202	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	601	4	-	0/6/23/26	0/1/1/1
4	NAG	D	602	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	603	4	-	0/6/23/26	0/1/1/1
4	NAG	D	604	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	201	2,4	-	0/6/23/26	0/1/1/1
4	NAG	E	202	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	203	NAG	C2-N2-C7	-2.69	119.59	123.04
4	E	201	NAG	C2-N2-C7	-2.61	119.69	123.04
4	D	604	NAG	C2-N2-C7	-2.57	119.74	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	201	NAG	C2-N2-C7	-2.46	119.88	123.04
4	B	201	NAG	C2-N2-C7	-2.41	119.94	123.04
4	B	202	NAG	C2-N2-C7	-2.40	119.95	123.04
4	D	603	NAG	C2-N2-C7	-2.29	120.10	123.04
4	A	204	NAG	C2-N2-C7	-2.27	120.12	123.04
4	A	202	NAG	C2-N2-C7	-2.19	120.23	123.04
4	D	601	NAG	C2-N2-C7	-2.19	120.23	123.04
4	E	202	NAG	C2-N2-C7	-2.17	120.25	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	201	NAG	1	0
4	A	202	NAG	1	0
4	A	204	NAG	2	0
4	D	601	NAG	2	0
4	D	602	NAG	2	0
4	D	603	NAG	3	0
4	D	604	NAG	2	0
4	E	201	NAG	1	0
4	E	202	NAG	1	0

5.6 Ligand geometry

4 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	$\# Z > 2$
5	IPA	A	205	-	3,3,3	0.69	0	3,3,3	0.33	0
5	IPA	A	206	-	3,3,3	0.63	0	3,3,3	0.33	0
5	IPA	B	203	-	3,3,3	0.66	0	3,3,3	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	IPA	E	203	-	3,3,3	0.64	0	3,3,3	0.32	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	IPA	A	205	-	-	0/0/0/0	0/0/0/0
5	IPA	A	206	-	-	0/0/0/0	0/0/0/0
5	IPA	B	203	-	-	0/0/0/0	0/0/0/0
5	IPA	E	203	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	205	IPA	2	0
5	B	203	IPA	1	0
5	E	203	IPA	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	180/180 (100%)	0.14	5 (2%)	56 55	22, 37, 74, 115	0
1	D	180/180 (100%)	0.45	14 (7%)	16 15	23, 48, 89, 128	0
2	B	188/188 (100%)	0.04	3 (1%)	74 73	21, 31, 62, 93	0
2	E	182/188 (96%)	0.33	9 (4%)	33 33	27, 45, 73, 103	0
3	C	22/22 (100%)	0.30	2 (9%)	11 11	22, 43, 66, 102	0
3	F	22/22 (100%)	0.29	2 (9%)	11 11	25, 37, 72, 98	0
All	All	774/780 (99%)	0.24	35 (4%)	37 36	21, 40, 78, 128	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	ALA	11.3
1	D	182	ALA	8.5
1	D	181	ASP	5.8
1	D	100	ARG	4.5
2	E	165	PRO	4.1
3	F	327	ARG	3.7
2	E	190	ALA	3.7
2	B	109	LEU	3.6
2	E	105	LYS	3.6
1	D	174	LEU	3.1
2	E	140	THR	3.0
2	E	53	LEU	2.8
1	D	175	LEU	2.7
1	A	158	GLU	2.6
2	B	111	HIS	2.6
3	C	327	ARG	2.6
1	D	171	ASP	2.6
1	A	100	ARG	2.5
3	F	325	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	98	GLU	2.4
2	E	181	THR	2.4
1	A	98	GLU	2.4
2	B	3	THR	2.3
1	D	126	LYS	2.3
1	A	40	GLU	2.3
2	E	113	ASN	2.3
3	C	306	GLN	2.2
1	D	96	PRO	2.2
2	E	182	SER	2.2
1	D	97	VAL	2.2
1	D	160	VAL	2.1
1	D	168	TRP	2.1
1	D	158	GLU	2.1
1	D	51	PHE	2.1
2	E	96	HIS	2.1

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](#)

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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	D	602	14/15	0.84	0.24	1.45	81,88,90,94	0
4	NAG	A	204	14/15	0.93	0.13	-0.07	51,56,61,68	0
4	NAG	E	201	14/15	0.73	0.28	-	103,112,116,125	0
4	NAG	A	201	14/15	0.43	0.74	-	179,190,193,193	0
4	NAG	B	201	14/15	0.66	0.36	-	127,132,134,134	0
4	NAG	B	202	14/15	0.58	0.30	-	100,109,112,119	0
4	NAG	D	601	14/15	0.74	0.33	-	99,102,103,104	0
4	NAG	A	203	14/15	0.77	0.28	-	75,79,81,81	0
4	NAG	D	603	14/15	0.49	0.38	-	143,148,149,149	0
4	NAG	A	202	14/15	0.60	0.39	-	129,139,148,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	D	604	14/15	0.50	0.39	-	117,128,130,137	0
4	NAG	E	202	14/15	0.51	0.50	-	134,141,142,143	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
5	IPA	A	205	4/4	0.78	0.25	3.42	40,41,43,44	0
5	IPA	E	203	4/4	0.83	0.22	2.39	43,44,45,46	0
5	IPA	B	203	4/4	0.58	0.27	1.85	39,40,42,43	0
5	IPA	A	206	4/4	0.86	0.17	0.36	45,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.