



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:30 PM GMT

PDB ID : 1KLG
Title : Crystal structure of HLA-DR1/TPI(23-37, Thr28->Ile mutant) complexed with staphylococcal enterotoxin C3 variant 3B2 (SEC3-3B2)
Authors : Sundberg, E.J.; Sawicki, M.W.; Andersen, P.S.; Sidney, J.; Sette, A.; Mariuzza, R.A.
Deposited on : 2001-12-11
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
<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

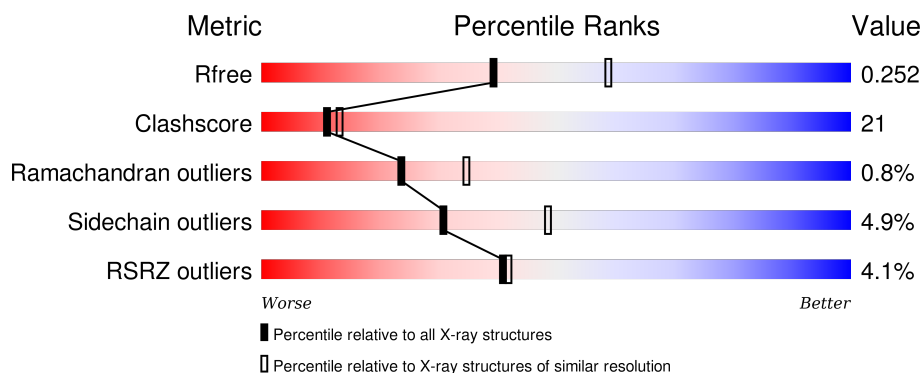
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 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	177	<div> <div>2%</div> <div>68%</div> <div>30%</div> <div>.</div> </div>
2	B	190	<div> <div>5%</div> <div>55%</div> <div>37%</div> <div>6%</div> <div>.</div> </div>
3	C	15	<div> <div>13%</div> <div>60%</div> <div>20%</div> <div>20%</div> </div>
4	D	239	<div> <div>4%</div> <div>67%</div> <div>27%</div> <div>.</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5260 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	177	Total	C	N	O	S	0	0	0
			1457	945	237	270	5			

- Molecule 2 is a protein called HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR-1 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	187	Total	C	N	O	S	0	0	0
			1533	963	275	289	6			

- Molecule 3 is a protein called Triosephosphate isomerase peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	0	0	0
			104	66	17	21			

- Molecule 4 is a protein called ENTEROTOXIN TYPE C-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	231	Total	C	N	O	S	0	0	0
			1891	1201	308	372	10			

There are 4 discrepancies between the modelled and reference sequences:

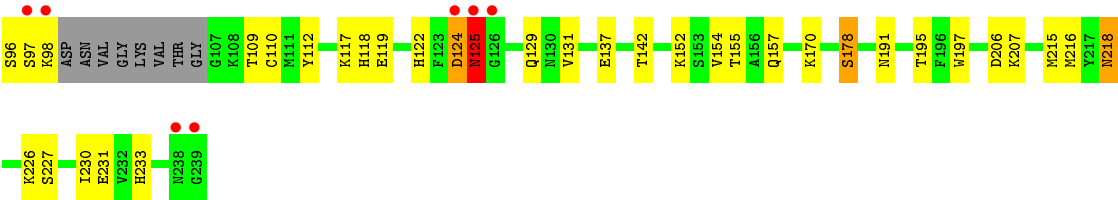
Chain	Residue	Modelled	Actual	Comment	Reference
D	43	SER	LYS	ENGINEERED	UNP P0A0L5
D	45	PHE	LEU	ENGINEERED	UNP P0A0L5
D	46	LYS	ALA	ENGINEERED	UNP P0A0L5
D	47	TRP	HIS	ENGINEERED	UNP P0A0L5

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	91	Total 91	O 91	0	0
5	B	67	Total 67	O 67	0	0
5	C	15	Total 15	O 15	0	0
5	D	102	Total 102	O 102	0	0

- Molecule 1: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN, DR ALPHA CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	172.99Å 172.99Å 121.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.96 – 2.40 36.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	80.5 (14.96-2.40) 93.3 (36.66-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.206 , 0.246 0.219 , 0.252	Depositor DCC
R_{free} test set	2644 reflections (5.66%)	DCC
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.8	EDS
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 52723 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5260	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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](#)

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	0.43	0/1502	0.70	0/2047
2	B	0.40	0/1571	0.64	0/2130
3	C	1.32	2/104 (1.9%)	1.31	2/139 (1.4%)
4	D	0.37	0/1933	0.61	0/2601
All	All	0.44	2/5110 (0.0%)	0.67	2/6917 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	27	GLY	C-N	9.54	1.55	1.34
3	C	28	ILE	C-N	-7.86	1.16	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	28	ILE	O-C-N	-10.03	106.66	122.70
3	C	28	ILE	CA-C-N	6.83	132.24	117.20

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	1457	0	1397	62	0
2	B	1533	0	1461	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	104	0	108	12	0
4	D	1891	0	1822	55	0
5	A	91	0	0	3	0
5	B	67	0	0	1	0
5	C	15	0	0	1	0
5	D	102	0	0	1	0
All	All	5260	0	4788	203	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 21.

All (203) 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)
2:B:127:ILE:HD11	2:B:175:VAL:HG13	1.19	1.15
1:A:82:ILE:HD13	2:B:33:ASN:HB3	1.17	1.12
2:B:150:ASN:HD22	2:B:154:THR:HG22	1.19	1.05
2:B:127:ILE:HD13	2:B:128:GLU:N	1.79	0.96
2:B:129:VAL:HG21	2:B:159:VAL:HG21	1.49	0.92
1:A:82:ILE:HD12	1:A:83:THR:H	1.35	0.91
2:B:127:ILE:HD11	2:B:175:VAL:CG1	2.03	0.89
4:D:46:LYS:HB3	4:D:71:GLU:HG3	1.54	0.88
2:B:114:LEU:HD21	2:B:160:MET:HB3	1.58	0.84
2:B:116:VAL:HG13	2:B:160:MET:HE1	1.61	0.82
1:A:22:PHE:CZ	3:C:28:ILE:HD11	2.16	0.80
2:B:150:ASN:ND2	2:B:154:THR:HG22	1.95	0.80
2:B:105:LYS:HE3	2:B:105:LYS:H	1.46	0.79
4:D:88:ASN:H	4:D:88:ASN:HD22	1.29	0.78
1:A:82:ILE:CD1	2:B:33:ASN:HB3	2.08	0.78
2:B:21:THR:O	2:B:80:ARG:NH1	2.18	0.76
4:D:215:MET:O	4:D:218:ASN:HB2	1.86	0.75
1:A:94:ASN:HD22	1:A:104:VAL:HB	1.52	0.74
2:B:31:ILE:CD1	2:B:36:GLU:HA	2.17	0.74
2:B:127:ILE:HD13	2:B:128:GLU:H	1.50	0.74
2:B:129:VAL:CG2	2:B:159:VAL:HG21	2.18	0.73
2:B:85:VAL:HG13	3:C:24:GLU:HB2	1.72	0.72
4:D:87:SER:H	4:D:157:GLN:HE21	1.35	0.72
1:A:7:ILE:HD13	2:B:17:PHE:CE2	2.24	0.72
2:B:31:ILE:HD13	2:B:36:GLU:HA	1.72	0.71
4:D:64:VAL:HG22	4:D:109:THR:HG22	1.72	0.69
4:D:117:LYS:HE2	4:D:119:GLU:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:ASP:OD1	2:B:154:THR:HB	1.92	0.69
1:A:109:ILE:HD12	1:A:165:VAL:HG21	1.74	0.69
2:B:8:LEU:O	2:B:32:TYR:O	2.11	0.68
1:A:129:THR:O	1:A:132:VAL:HG22	1.95	0.67
1:A:82:ILE:HD12	1:A:83:THR:N	2.08	0.67
2:B:94:ARG:HH11	2:B:94:ARG:HG3	1.60	0.66
1:A:16:PRO:HD2	2:B:6:ARG:HD3	1.77	0.66
4:D:87:SER:H	4:D:157:GLN:NE2	1.92	0.66
1:A:147:LYS:HE3	1:A:149:HIS:HE1	1.62	0.65
2:B:86:GLY:HA2	2:B:89:PHE:CE1	2.32	0.65
4:D:64:VAL:HG22	4:D:109:THR:CG2	2.27	0.64
2:B:2:ASP:CG	2:B:6:ARG:HH22	2.01	0.64
2:B:106:THR:O	2:B:107:GLN:O	2.16	0.64
1:A:82:ILE:HD13	2:B:33:ASN:CB	2.11	0.64
2:B:105:LYS:CE	2:B:105:LYS:H	2.10	0.63
1:A:7:ILE:HD13	2:B:17:PHE:HE2	1.62	0.63
4:D:57:LYS:HB3	4:D:58:LEU:HD22	1.81	0.63
2:B:116:VAL:HG13	2:B:160:MET:CE	2.30	0.62
2:B:150:ASN:HD22	2:B:154:THR:CG2	2.04	0.62
2:B:13:PHE:CD2	3:C:29:LEU:HD23	2.35	0.62
1:A:36:MET:HG2	4:D:45:PHE:CZ	2.35	0.61
4:D:76:LYS:HD2	4:D:77:TYR:CE1	2.36	0.61
1:A:89:VAL:HG13	1:A:109:ILE:HD13	1.81	0.61
4:D:122:HIS:O	4:D:152:LYS:HE3	2.00	0.61
2:B:23:ARG:HG2	2:B:23:ARG:HH21	1.63	0.61
2:B:2:ASP:OD1	2:B:4:ARG:HD3	2.00	0.61
2:B:70:GLN:HG3	2:B:71:ARG:N	2.16	0.61
2:B:93:ARG:O	2:B:94:ARG:HG3	2.01	0.60
1:A:22:PHE:CE2	3:C:28:ILE:HD11	2.35	0.60
1:A:72:ILE:HG13	5:A:270:HOH:O	2.02	0.60
2:B:145:THR:HG22	2:B:158:LEU:H	1.65	0.60
2:B:30:CYS:O	2:B:31:ILE:HD13	2.02	0.60
1:A:95:SER:HB2	1:A:96:PRO:HD2	1.84	0.60
2:B:28:GLU:HB3	2:B:40:PHE:HB3	1.85	0.59
4:D:58:LEU:HD22	4:D:58:LEU:N	2.18	0.58
4:D:231:GLU:HB3	4:D:233:HIS:CE1	2.39	0.58
1:A:73:MET:HG3	2:B:9:TRP:CZ3	2.39	0.57
5:A:270:HOH:O	3:C:34:VAL:HG22	2.04	0.57
1:A:143:HIS:HD2	2:B:12:LYS:NZ	2.02	0.57
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.86	0.57
4:D:191:ASN:HB3	4:D:227:SER:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:VAL:N	2:B:160:MET:HE3	2.20	0.57
4:D:231:GLU:HB3	4:D:233:HIS:HE1	1.70	0.56
2:B:111:HIS:CG	2:B:112:HIS:H	2.24	0.56
2:B:65:LYS:HD2	2:B:65:LYS:H	1.70	0.56
1:A:13:TYR:CZ	1:A:67:LYS:HD2	2.41	0.56
2:B:31:ILE:HD12	2:B:36:GLU:HA	1.86	0.56
1:A:94:ASN:ND2	1:A:104:VAL:HB	2.20	0.55
1:A:109:ILE:CD1	1:A:165:VAL:HG21	2.37	0.55
1:A:76:ARG:HH22	2:B:57:ASP:CG	2.09	0.55
4:D:88:ASN:H	4:D:88:ASN:ND2	2.02	0.55
2:B:161:LEU:HG	2:B:163:THR:HG23	1.89	0.55
1:A:107:CYS:HB2	1:A:121:TRP:CH2	2.42	0.55
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.89	0.54
2:B:31:ILE:HD12	2:B:36:GLU:CA	2.37	0.54
1:A:89:VAL:HG13	1:A:109:ILE:CD1	2.38	0.53
3:C:34:VAL:HB	3:C:35:PRO:HD2	1.91	0.53
1:A:36:MET:HG2	4:D:45:PHE:CE1	2.43	0.53
1:A:73:MET:CE	2:B:53:LEU:HD13	2.39	0.53
4:D:6:PRO:HD3	4:D:197:TRP:CE2	2.44	0.53
2:B:29:ARG:NH2	2:B:36:GLU:OE1	2.40	0.52
2:B:94:ARG:NH1	2:B:94:ARG:HG3	2.23	0.52
2:B:161:LEU:HG	2:B:163:THR:CG2	2.40	0.52
1:A:107:CYS:SG	1:A:109:ILE:HD11	2.50	0.51
2:B:107:GLN:HE21	2:B:114:LEU:H	1.59	0.51
2:B:114:LEU:CD2	2:B:160:MET:HB3	2.34	0.51
2:B:166:ARG:N	2:B:169:GLU:OE1	2.44	0.51
2:B:127:ILE:HD12	2:B:129:VAL:CG1	2.41	0.51
4:D:42:ASP:OD1	4:D:97:SER:HA	2.11	0.50
2:B:93:ARG:HG2	2:B:123:TYR:CD1	2.47	0.50
2:B:52:GLU:OE1	2:B:55:ARG:HD2	2.11	0.50
4:D:6:PRO:HB3	4:D:197:TRP:CZ2	2.47	0.50
2:B:116:VAL:HG22	2:B:160:MET:HG3	1.94	0.50
5:B:217:HOH:O	3:C:27:GLY:HA3	2.11	0.50
2:B:166:ARG:O	2:B:169:GLU:HG3	2.13	0.49
2:B:57:ASP:OD1	3:C:34:VAL:HB	2.13	0.49
4:D:110:CYS:HB3	5:D:242:HOH:O	2.11	0.49
1:A:98:GLU:HB2	1:A:101:GLU:HG3	1.94	0.48
2:B:130:ARG:HB2	2:B:132:PHE:HE1	1.77	0.48
2:B:145:THR:CG2	2:B:158:LEU:H	2.25	0.48
2:B:127:ILE:HG12	2:B:177:HIS:HB2	1.96	0.48
2:B:31:ILE:CD1	2:B:36:GLU:CA	2.89	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:97:SER:O	4:D:98:LYS:HB2	2.13	0.48
2:B:18:PHE:N	2:B:18:PHE:CD1	2.80	0.48
4:D:33:VAL:O	4:D:85:TYR:HA	2.14	0.48
2:B:129:VAL:HG21	2:B:159:VAL:CG2	2.32	0.48
4:D:124:ASP:O	4:D:125:ASN:CB	2.62	0.48
1:A:81:PRO:HB3	2:B:5:PRO:HB2	1.94	0.48
4:D:131:VAL:CG1	4:D:230:ILE:HD13	2.43	0.48
4:D:83:ASP:OD1	4:D:118:HIS:HD2	1.97	0.48
2:B:118:SER:HA	2:B:158:LEU:HD23	1.96	0.48
2:B:158:LEU:HB3	2:B:160:MET:CE	2.43	0.48
4:D:216:MET:C	4:D:218:ASN:H	2.17	0.47
4:D:97:SER:O	4:D:98:LYS:CB	2.62	0.47
1:A:122:LEU:HD23	1:A:127:PRO:HA	1.96	0.47
4:D:6:PRO:HB3	4:D:197:TRP:CH2	2.49	0.47
4:D:39:LYS:HB2	4:D:39:LYS:NZ	2.29	0.47
4:D:54:SER:HA	4:D:62:ASP:HA	1.97	0.47
1:A:10:ALA:HB3	1:A:23:MET:HE2	1.95	0.47
2:B:129:VAL:HA	2:B:174:GLN:O	2.15	0.47
1:A:22:PHE:CG	1:A:59:ALA:HB1	2.50	0.47
4:D:42:ASP:HB3	4:D:50:ILE:HB	1.96	0.47
1:A:42:VAL:HG22	1:A:42:VAL:O	2.13	0.47
4:D:2:SER:HB2	4:D:195:THR:H	1.80	0.47
4:D:96:SER:O	4:D:97:SER:HB3	2.15	0.47
1:A:17:ASP:O	1:A:18:GLN:HG2	2.15	0.46
1:A:118:ASN:HB3	1:A:166:GLU:HB2	1.96	0.46
2:B:121:GLY:HA2	2:B:154:THR:HG23	1.97	0.46
1:A:36:MET:HG3	1:A:60:LEU:CD1	2.46	0.46
1:A:36:MET:HG3	1:A:60:LEU:HD11	1.97	0.46
4:D:21:MET:CB	4:D:178:SER:H	2.29	0.46
1:A:74:THR:HA	2:B:32:TYR:OH	2.16	0.46
2:B:78:TYR:CD2	3:C:29:LEU:HD22	2.50	0.46
4:D:94:TYR:O	4:D:95:PHE:HB3	2.16	0.46
1:A:12:PHE:HB3	2:B:10:GLN:HG2	1.98	0.46
1:A:124:ASN:OD1	1:A:160:VAL:HG22	2.15	0.46
2:B:65:LYS:HD2	2:B:65:LYS:N	2.31	0.46
1:A:171:ASP:O	1:A:172:GLU:HG3	2.15	0.46
2:B:57:ASP:OD1	3:C:35:PRO:HD2	2.16	0.45
1:A:70:LEU:HD13	2:B:9:TRP:HB2	1.98	0.45
4:D:129:GLN:OE1	4:D:226:LYS:HA	2.16	0.45
1:A:76:ARG:NH2	2:B:57:ASP:OD2	2.50	0.45
2:B:158:LEU:HB3	2:B:160:MET:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:18:THR:HB	4:D:206:ASP:HA	1.99	0.45
4:D:59:LYS:HA	4:D:59:LYS:HE2	1.98	0.45
4:D:119:GLU:HA	4:D:119:GLU:OE2	2.17	0.45
4:D:21:MET:HB2	4:D:178:SER:H	1.81	0.45
2:B:176:GLU:HG2	2:B:183:PRO:HB3	1.99	0.45
1:A:22:PHE:CZ	3:C:28:ILE:CD1	2.95	0.45
2:B:130:ARG:NH1	2:B:174:GLN:HE21	2.15	0.45
1:A:122:LEU:HB2	1:A:162:ASP:HB2	1.98	0.45
4:D:68:LEU:HB3	4:D:73:LEU:HD23	1.99	0.44
4:D:137:GLU:HB2	4:D:142:THR:HG21	1.99	0.44
4:D:31:HIS:O	4:D:32:TYR:HB3	2.17	0.44
4:D:88:ASN:HA	4:D:110:CYS:O	2.17	0.44
1:A:17:ASP:C	1:A:18:GLN:HG2	2.38	0.44
2:B:137:GLU:HG2	2:B:139:LYS:HE3	2.00	0.44
2:B:129:VAL:HG23	2:B:129:VAL:O	2.16	0.44
1:A:110:ASP:OD1	1:A:140:ARG:HD2	2.17	0.44
4:D:25:LYS:HE2	4:D:29:ASP:OD1	2.18	0.43
4:D:91:VAL:O	4:D:92:ASN:HB2	2.18	0.43
1:A:73:MET:HE1	2:B:53:LEU:HD22	1.99	0.43
1:A:162:ASP:HA	1:A:176:LYS:O	2.17	0.43
1:A:10:ALA:HB3	1:A:23:MET:CE	2.48	0.43
2:B:115:LEU:O	2:B:160:MET:HA	2.18	0.43
2:B:158:LEU:C	2:B:160:MET:HE3	2.39	0.43
2:B:23:ARG:HG2	2:B:23:ARG:NH2	2.32	0.43
1:A:143:HIS:HD2	2:B:12:LYS:HZ2	1.64	0.43
2:B:31:ILE:CD1	2:B:36:GLU:CB	2.96	0.43
1:A:36:MET:CE	1:A:63:ILE:HG13	2.48	0.43
4:D:112:TYR:CE2	4:D:215:MET:HG3	2.54	0.43
4:D:170:LYS:HA	4:D:170:LYS:HD3	1.92	0.43
4:D:86:GLY:CA	4:D:157:GLN:NE2	2.82	0.42
2:B:129:VAL:CG2	2:B:129:VAL:O	2.66	0.42
2:B:65:LYS:HE2	2:B:65:LYS:HA	2.01	0.42
4:D:3:GLN:HA	4:D:4:PRO:HD3	1.84	0.42
1:A:9:GLN:HG3	1:A:24:PHE:CE1	2.55	0.42
2:B:166:ARG:O	2:B:167:SER:C	2.59	0.42
4:D:39:LYS:CB	4:D:39:LYS:NZ	2.83	0.41
2:B:130:ARG:HB2	2:B:132:PHE:CE1	2.54	0.41
2:B:177:HIS:CG	2:B:178:PRO:HD2	2.55	0.41
2:B:31:ILE:HD12	2:B:36:GLU:CB	2.50	0.41
2:B:31:ILE:HD12	2:B:36:GLU:HB2	2.02	0.41
3:C:29:LEU:HD12	3:C:29:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:TRP:HB3	2:B:161:LEU:HD22	2.02	0.41
1:A:42:VAL:O	1:A:42:VAL:CG2	2.67	0.41
2:B:2:ASP:OD1	2:B:6:ARG:NH2	2.53	0.41
2:B:90:THR:OG1	2:B:91:VAL:N	2.54	0.41
1:A:76:ARG:HB3	5:C:275:HOH:O	2.19	0.41
2:B:111:HIS:CG	2:B:112:HIS:N	2.89	0.41
4:D:154:VAL:HG22	4:D:155:THR:N	2.36	0.41
1:A:72:ILE:CG1	5:A:270:HOH:O	2.66	0.40
1:A:60:LEU:HD22	1:A:60:LEU:N	2.36	0.40
1:A:12:PHE:CD1	1:A:12:PHE:C	2.94	0.40
1:A:122:LEU:O	1:A:161:TYR:HA	2.21	0.40
4:D:131:VAL:HG11	4:D:230:ILE:HD13	2.04	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	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
2	B	183/190 (96%)	173 (94%)	9 (5%)	1 (0%)	34	48
3	C	13/15 (87%)	13 (100%)	0	0	100	100
4	D	227/239 (95%)	212 (93%)	11 (5%)	4 (2%)	11	13
All	All	598/621 (96%)	565 (94%)	28 (5%)	5 (1%)	24	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	57	LYS
4	D	125	ASN
4	D	124	ASP

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Mol	Chain	Res	Type
2	B	32	TYR
4	D	178	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/162 (100%)	157 (97%)	5 (3%)	47	69
2	B	168/171 (98%)	151 (90%)	17 (10%)	9	13
3	C	10/10 (100%)	9 (90%)	1 (10%)	9	14
4	D	213/220 (97%)	209 (98%)	4 (2%)	65	83
All	All	553/563 (98%)	526 (95%)	27 (5%)	31	48

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	23	MET
1	A	36	MET
1	A	82	ILE
1	A	146	ARG
2	B	18	PHE
2	B	23	ARG
2	B	29	ARG
2	B	35	GLU
2	B	38	VAL
2	B	53	LEU
2	B	59	GLU
2	B	65	LYS
2	B	68	LEU
2	B	69	GLU
2	B	70	GLN
2	B	71	ARG
2	B	98	LYS
2	B	105	LYS

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Mol	Chain	Res	Type
2	B	114	LEU
2	B	127	ILE
2	B	160	MET
3	C	24	GLU
4	D	88	ASN
4	D	125	ASN
4	D	207	LYS
4	D	218	ASN

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	118	ASN
1	A	143	HIS
1	A	149	HIS
2	B	19	ASN
2	B	92	GLN
2	B	107	GLN
2	B	113	ASN
2	B	134	ASN
2	B	150	ASN
2	B	156	GLN
2	B	174	GLN
4	D	60	ASN
4	D	88	ASN
4	D	92	ASN
4	D	125	ASN
4	D	129	GLN
4	D	157	GLN
4	D	218	ASN
4	D	233	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	177/177 (100%)	-0.13	4 (2%) 64 63	12, 25, 51, 63	0
2	B	187/190 (98%)	0.01	10 (5%) 30 30	13, 33, 66, 86	0
3	C	15/15 (100%)	0.37	2 (13%) 4 4	19, 26, 61, 64	0
4	D	231/239 (96%)	-0.15	9 (3%) 43 44	16, 31, 64, 75	0
All	All	610/621 (98%)	-0.08	25 (4%) 41 42	12, 31, 62, 86	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	106	THR	4.3
2	B	111	HIS	4.1
4	D	125	ASN	4.1
3	C	24	GLU	3.7
4	D	124	ASP	3.6
3	C	23	GLY	3.4
2	B	112	HIS	3.2
4	D	58	LEU	3.1
2	B	107	GLN	3.0
4	D	239	GLY	2.8
4	D	97	SER	2.8
1	A	158	GLU	2.7
2	B	1	GLY	2.7
2	B	139	LYS	2.7
2	B	166	ARG	2.7
1	A	129	THR	2.7
4	D	126	GLY	2.6
1	A	130	THR	2.6
4	D	238	ASN	2.5
2	B	140	ALA	2.3
4	D	56	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	136	GLN	2.3
1	A	126	LYS	2.2
2	B	164	VAL	2.1
4	D	98	LYS	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](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.