



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2017 – 10:32 PM EDT

PDB ID : 5WKI
Title : Crystal structure of PG90 TCR-CD1b-PG complex
Authors : Shahine, A.; Gras, S.; Rossjohn, J.
Deposited on : unknown
Resolution : 2.75 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

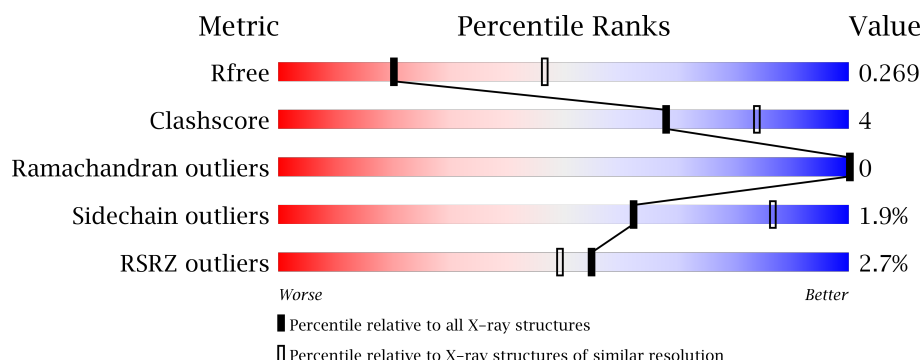
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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	300	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>11%</div> </div> </div>
2	B	99	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>
3	D	204	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>.</div> </div> </div>
4	E	249	<div> <div></div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	D3D	D	308	-	-	-	X
11	ACT	E	302	-	-	X	-
5	CUY	A	401	-	-	-	X

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 6732 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 surface glycoprotein CD1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2069	1328	351	380	10			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	GLY	-	expression tag	UNP P29016
A	280	SER	-	expression tag	UNP P29016
A	281	GLY	-	expression tag	UNP P29016
A	282	LEU	-	expression tag	UNP P29016
A	283	ASN	-	expression tag	UNP P29016
A	284	ASP	-	expression tag	UNP P29016
A	285	ILE	-	expression tag	UNP P29016
A	286	PHE	-	expression tag	UNP P29016
A	287	GLU	-	expression tag	UNP P29016
A	288	ALA	-	expression tag	UNP P29016
A	289	GLN	-	expression tag	UNP P29016
A	290	LYS	-	expression tag	UNP P29016
A	291	ILE	-	expression tag	UNP P29016
A	292	GLU	-	expression tag	UNP P29016
A	293	TRP	-	expression tag	UNP P29016
A	294	HIS	-	expression tag	UNP P29016
A	295	GLU	-	expression tag	UNP P29016
A	296	HIS	-	expression tag	UNP P29016
A	297	HIS	-	expression tag	UNP P29016
A	298	HIS	-	expression tag	UNP P29016
A	299	HIS	-	expression tag	UNP P29016
A	300	HIS	-	expression tag	UNP P29016
A	301	HIS	-	expression tag	UNP P29016

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			790	504	135	149	2			

- Molecule 3 is a protein called T-cell receptor alpha variable 26-1,TRA@ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	198	Total	C	N	O	S	0	0	0
			1539	958	263	308	10			

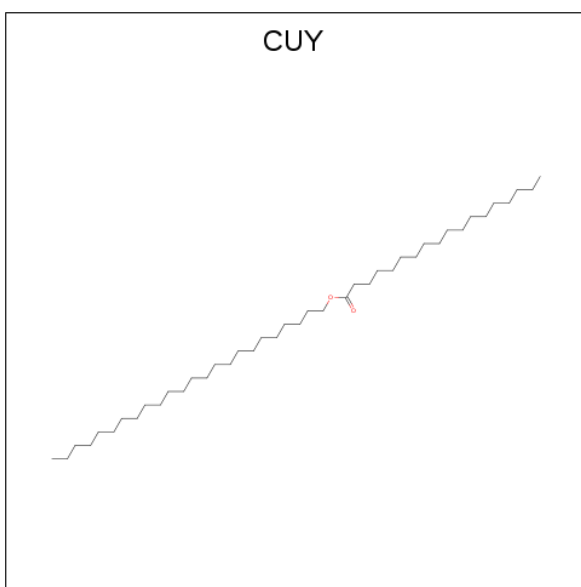
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	8	PRO	THR	conflict	UNP A0A087WT03
D	91	ARG	-	linker	UNP A0A087WT03
D	92	VAL	-	linker	UNP A0A087WT03
D	93	ALA	-	linker	UNP A0A087WT03
D	94	TYR	-	linker	UNP A0A087WT03
D	95	ARG	-	linker	UNP A0A087WT03
D	96	GLN	-	linker	UNP A0A087WT03
D	97	LYS	-	linker	UNP A0A087WT03
D	98	VAL	-	linker	UNP A0A087WT03
D	99	THR	-	linker	UNP A0A087WT03
D	100	PHE	-	linker	UNP A0A087WT03
D	101	GLY	-	linker	UNP A0A087WT03
D	102	THR	-	linker	UNP A0A087WT03
D	103	GLY	-	linker	UNP A0A087WT03
D	104	THR	-	linker	UNP A0A087WT03
D	105	LYS	-	linker	UNP A0A087WT03
D	106	LEU	-	linker	UNP A0A087WT03
D	107	GLN	-	linker	UNP A0A087WT03
D	108	VAL	-	linker	UNP A0A087WT03
D	109	ILE	-	linker	UNP A0A087WT03
D	110	PRO	-	linker	UNP A0A087WT03
D	158	CYS	THR	conflict	UNP Q6P4G7

- Molecule 4 is a protein called PG90 TCR beta chain.

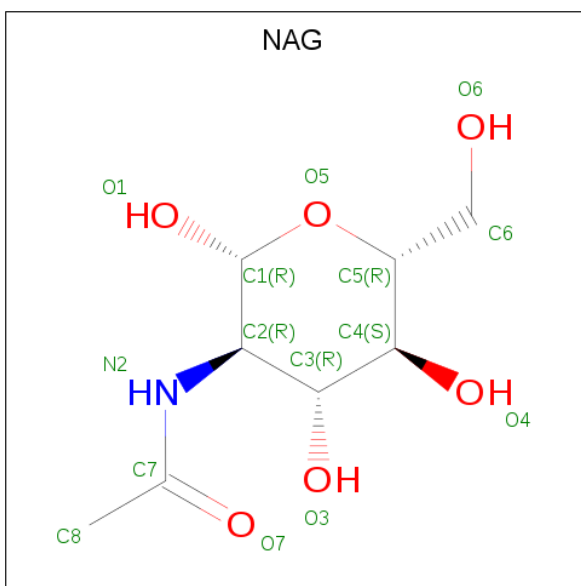
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	248	Total	C	N	O	S	0	0	0
			1954	1229	345	375	5			

- Molecule 5 is tetracosyl octadecanoate (three-letter code: CUY) (formula: C₄₂H₈₄O₂).



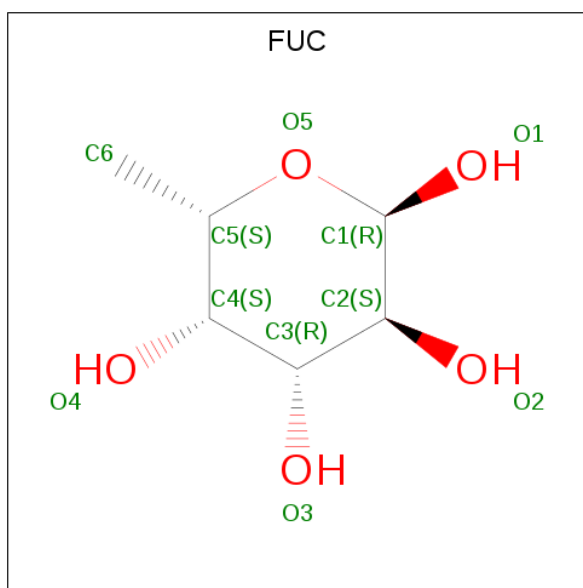
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			23	21	2		

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



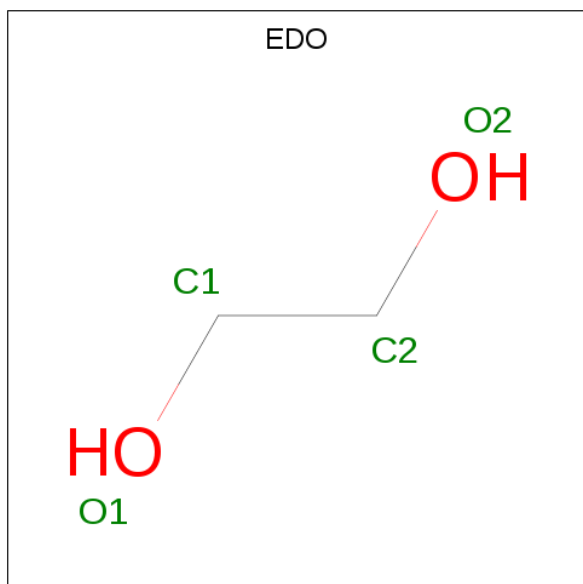
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	5	0
			14	8	1	5		

- Molecule 7 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	4	0
			10	6	4		
7	A	1	Total	C	O	4	0
			10	6	4		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		

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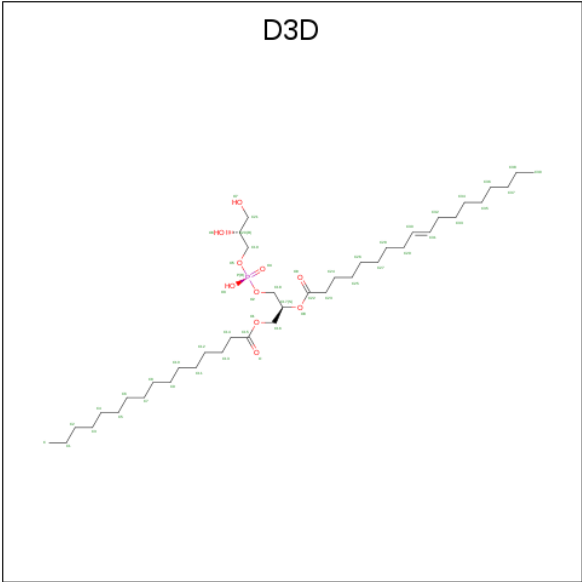
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0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

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

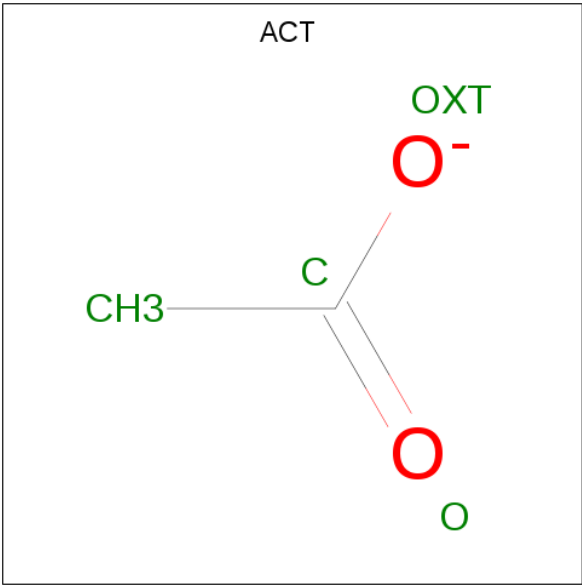
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total Na 1 1	0	0
9	E	1	Total Na 1 1	0	0

- Molecule 10 is (19S,22R,25R)-22,25,26-trihydroxy-16,22-dioxo-17,21,23-trioxa-22lambda 5 -phosphahexacosan-19-yl (9E)-octadec-9-enoate (three-letter code: D3D) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 11 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	E	1	Total	C	O	0	0
			4	2	2		
11	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	E	1	Total Cl 1 1	0	0

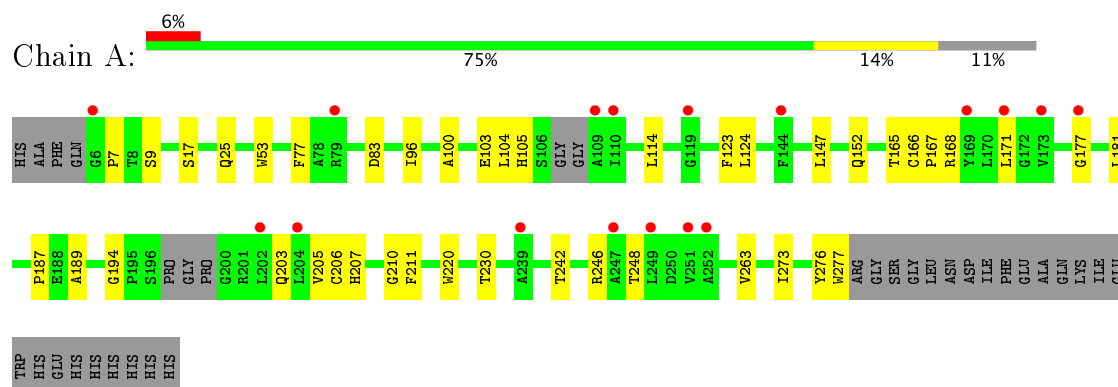
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	45	Total O 45 45	0	0
13	B	17	Total O 17 17	0	0
13	D	47	Total O 47 47	0	0
13	E	78	Total O 78 78	0	0

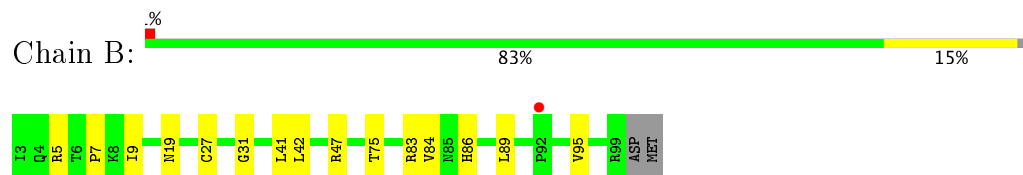
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

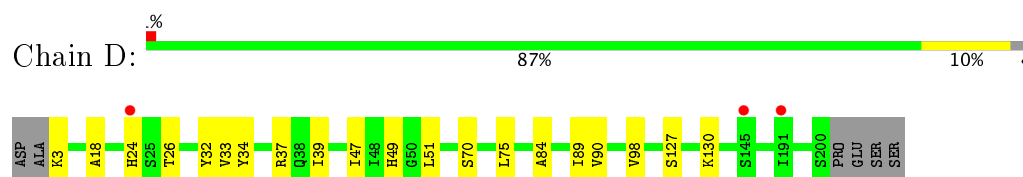
- Molecule 1: T-cell surface glycoprotein CD1b



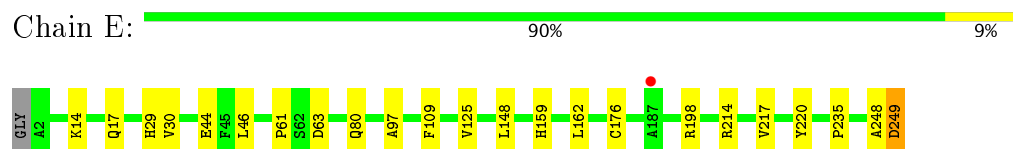
- Molecule 2: Beta-2-microglobulin



- Molecule 3: T-cell receptor alpha variable 26-1, TRA@ protein



- Molecule 4: PG90 TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.01 Å 82.97 Å 90.16 Å 90.00° 94.88° 90.00°	Depositor
Resolution (Å)	75.73 – 2.75 75.73 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (75.73-2.75) 99.8 (75.73-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.73 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.212 , 0.252 0.223 , 0.269	Depositor DCC
R_{free} test set	1500 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6732	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: NAG, CL, NA, EDO, CUY, FUC, ACT, D3D

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	0.42	0/2122	0.63	0/2878
2	B	0.42	0/813	0.66	0/1106
3	D	0.46	0/1573	0.71	0/2144
4	E	0.43	0/2004	0.64	0/2724
All	All	0.43	0/6512	0.66	0/8852

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	2069	0	1988	24	0
2	B	790	0	730	10	0
3	D	1539	0	1451	11	0
4	E	1954	0	1861	12	0
5	A	23	0	0	0	0
6	A	42	0	36	0	0
7	A	20	0	20	0	0
8	A	20	0	30	1	0
8	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	24	0	36	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
10	D	49	0	0	0	0
11	E	8	0	6	3	0
12	E	1	0	0	0	0
13	A	45	0	0	1	0
13	B	17	0	0	0	0
13	D	47	0	0	0	0
13	E	78	0	0	1	0
All	All	6732	0	6164	56	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 (56) 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:100:ALA:HB2	1:A:114:LEU:HD23	1.61	0.80
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.69	0.74
1:A:104:LEU:HD21	13:A:540:HOH:O	1.94	0.68
2:B:7:PRO:HD2	2:B:89:LEU:HD21	1.81	0.63
3:D:37:ARG:HB2	3:D:47:ILE:HD11	1.83	0.60
1:A:276:TYR:O	1:A:277:TRP:HB2	2.01	0.59
4:E:248:ALA:O	4:E:249:ASP:HB2	2.00	0.59
1:A:220:TRP:H	1:A:230:THR:HG21	1.68	0.58
2:B:42:LEU:HD23	2:B:47:ARG:HA	1.85	0.56
3:D:39:ILE:HD13	3:D:84:ALA:HB2	1.92	0.52
1:A:206:CYS:O	1:A:246:ARG:HA	2.12	0.50
4:E:44:GLU:OE2	11:E:302:ACT:C	2.61	0.49
3:D:34:TYR:HB2	3:D:89:ILE:HG13	1.94	0.48
1:A:263:VAL:HB	1:A:273:ILE:HB	1.96	0.48
2:B:42:LEU:HD21	2:B:83:ARG:HH11	1.79	0.47
1:A:205:VAL:HG22	1:A:248:THR:HG22	1.97	0.47
1:A:220:TRP:HB2	1:A:230:THR:HG22	1.97	0.46
2:B:42:LEU:HD23	2:B:47:ARG:CA	2.45	0.46
3:D:3:LYS:HB3	3:D:24:HIS:CE1	2.50	0.46
1:A:165:THR:HG22	1:A:168:ARG:NH2	2.31	0.46
1:A:194:GLY:HA3	1:A:203:GLN:HB3	1.98	0.46
4:E:159:HIS:HB3	4:E:220:TYR:HB2	1.99	0.46
3:D:3:LYS:HB3	3:D:24:HIS:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ALA:HA	1:A:207:HIS:O	2.15	0.45
1:A:7:PRO:HG2	1:A:181:LEU:HD22	1.97	0.45
3:D:32:TYR:CD1	3:D:51:LEU:HB3	2.52	0.45
4:E:44:GLU:OE2	11:E:302:ACT:CH3	2.65	0.45
4:E:46:LEU:HD22	4:E:61:PRO:HD3	1.97	0.45
2:B:5:ARG:HB3	2:B:31:GLY:O	2.17	0.45
1:A:166:CYS:HB3	1:A:167:PRO:HD3	1.98	0.45
1:A:165:THR:HG22	1:A:168:ARG:HH21	1.82	0.44
1:A:17:SER:HB2	1:A:25:GLN:HG3	1.99	0.44
2:B:27:CYS:HB2	2:B:41:LEU:HD21	1.99	0.44
3:D:89:ILE:HD13	3:D:98:VAL:HG13	2.00	0.44
1:A:100:ALA:HB2	1:A:114:LEU:CD2	2.41	0.44
4:E:29:HIS:HE1	4:E:109:PHE:CD1	2.36	0.44
2:B:86:HIS:HB3	2:B:89:LEU:HG	1.99	0.43
4:E:214:ARG:HD3	13:E:404:HOH:O	2.18	0.43
1:A:53:TRP:CD2	1:A:177:GLY:HA3	2.52	0.43
1:A:152:GLN:HB3	3:D:51:LEU:HD21	2.00	0.43
4:E:14:LYS:HB3	4:E:17:GLN:HG3	2.00	0.43
2:B:19:ASN:OD1	2:B:75:THR:HA	2.17	0.43
2:B:9:ILE:HG12	2:B:84:VAL:HG21	2.01	0.42
1:A:207:HIS:HE1	8:A:407:EDO:C2	2.32	0.42
4:E:125:VAL:HG12	4:E:235:PRO:HB2	2.00	0.42
1:A:9:SER:HB3	1:A:103:GLU:HG3	2.02	0.42
4:E:30:VAL:HB	4:E:97:ALA:HB3	2.00	0.42
3:D:18:ALA:HB3	3:D:75:LEU:HB2	2.01	0.42
1:A:210:GLY:HA2	1:A:242:THR:HB	2.03	0.41
3:D:33:VAL:O	3:D:49:HIS:HA	2.21	0.41
4:E:44:GLU:OE2	11:E:302:ACT:H2	2.20	0.41
1:A:77:PHE:HZ	1:A:96:ILE:HG21	1.86	0.41
3:D:127:SER:OG	3:D:130:LYS:HG3	2.21	0.41
2:B:9:ILE:HB	2:B:95:VAL:HG21	2.03	0.41
1:A:123:PHE:HD1	1:A:124:LEU:HD23	1.86	0.40
4:E:162:LEU:HG	4:E:217:VAL:HG22	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	261/300 (87%)	252 (97%)	9 (3%)	0	100	100
2	B	95/99 (96%)	93 (98%)	2 (2%)	0	100	100
3	D	196/204 (96%)	187 (95%)	9 (5%)	0	100	100
4	E	246/249 (99%)	237 (96%)	9 (4%)	0	100	100
All	All	798/852 (94%)	769 (96%)	29 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	215/247 (87%)	211 (98%)	4 (2%)	62	87
2	B	86/94 (92%)	86 (100%)	0	100	100
3	D	174/184 (95%)	171 (98%)	3 (2%)	66	88
4	E	209/210 (100%)	203 (97%)	6 (3%)	48	78
All	All	684/735 (93%)	671 (98%)	13 (2%)	62	87

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

Mol	Chain	Res	Type
1	A	83	ASP
1	A	105	HIS

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Mol	Chain	Res	Type
1	A	147	LEU
1	A	171	LEU
3	D	26	THR
3	D	70	SER
3	D	90	VAL
4	E	63	ASP
4	E	80	GLN
4	E	148	LEU
4	E	176	CYS
4	E	198	ARG
4	E	249	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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
5	CUY	A	401	-	22,22,43	0.82	1 (4%)	22,22,43	0.99	1 (4%)
6	NAG	A	402	1	14,14,15	0.38	0	15,19,21	1.09	1 (6%)
7	FUC	A	403	6	9,10,11	0.34	0	13,14,16	1.11	2 (15%)
7	FUC	A	404	6	9,10,11	0.41	0	13,14,16	0.71	0
6	NAG	A	405	1,7,6	14,14,15	0.36	0	15,19,21	1.55	3 (20%)
6	NAG	A	406	6	14,14,15	0.34	0	15,19,21	1.18	3 (20%)
8	EDO	A	407	-	3,3,3	0.57	0	2,2,2	0.44	0
8	EDO	A	408	-	3,3,3	0.54	0	2,2,2	0.36	0
8	EDO	A	409	-	3,3,3	0.61	0	2,2,2	0.15	0
8	EDO	A	410	-	3,3,3	0.67	0	2,2,2	0.09	0
8	EDO	A	411	-	3,3,3	0.63	0	2,2,2	0.14	0
8	EDO	B	201	-	3,3,3	0.61	0	2,2,2	0.21	0
8	EDO	D	301	-	3,3,3	0.60	0	2,2,2	0.25	0
8	EDO	D	302	-	3,3,3	0.58	0	2,2,2	0.31	0
8	EDO	D	303	-	3,3,3	0.61	0	2,2,2	0.16	0
8	EDO	D	304	-	3,3,3	0.61	0	2,2,2	0.25	0
8	EDO	D	305	-	3,3,3	0.54	0	2,2,2	0.38	0
8	EDO	D	306	-	3,3,3	0.64	0	2,2,2	0.21	0
10	D3D	D	308	-	48,48,50	0.93	2 (4%)	49,54,56	1.09	1 (2%)
11	ACT	E	301	-	1,3,3	4.31	1 (100%)	0,3,3	0.00	-
11	ACT	E	302	-	1,3,3	5.03	1 (100%)	0,3,3	0.00	-

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	CUY	A	401	-	-	0/21/21/42	0/0/0/0
6	NAG	A	402	1	-	0/6/23/26	0/1/1/1
7	FUC	A	403	6	-	0/0/17/20	0/1/1/1
7	FUC	A	404	6	-	0/0/17/20	0/1/1/1
6	NAG	A	405	1,7,6	-	0/6/23/26	0/1/1/1
6	NAG	A	406	6	-	0/6/23/26	0/1/1/1
8	EDO	A	407	-	-	0/1/1/1	0/0/0/0
8	EDO	A	408	-	-	0/1/1/1	0/0/0/0
8	EDO	A	409	-	-	0/1/1/1	0/0/0/0
8	EDO	A	410	-	-	0/1/1/1	0/0/0/0
8	EDO	A	411	-	-	0/1/1/1	0/0/0/0
8	EDO	B	201	-	-	0/1/1/1	0/0/0/0
8	EDO	D	301	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	D	302	-	-	0/1/1/1	0/0/0/0
8	EDO	D	303	-	-	0/1/1/1	0/0/0/0
8	EDO	D	304	-	-	0/1/1/1	0/0/0/0
8	EDO	D	305	-	-	0/1/1/1	0/0/0/0
8	EDO	D	306	-	-	0/1/1/1	0/0/0/0
10	D3D	D	308	-	-	0/53/53/55	0/0/0/0
11	ACT	E	301	-	-	0/0/0/0	0/0/0/0
11	ACT	E	302	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	308	D3D	O8-C22	2.42	1.41	1.34
5	A	401	CUY	OAQ-CAP	2.85	1.41	1.33
10	D	308	D3D	O1-C15	2.96	1.42	1.33
11	E	301	ACT	CH3-C	4.31	1.54	1.48
11	E	302	ACT	CH3-C	5.03	1.55	1.48

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	405	NAG	O5-C1-C2	-3.92	106.02	111.47
6	A	406	NAG	O5-C1-C2	-2.12	108.53	111.47
6	A	405	NAG	C3-C4-C5	2.02	113.78	110.22
7	A	403	FUC	C3-C4-C5	2.12	113.02	109.68
7	A	403	FUC	C1-O5-C5	2.25	117.36	112.39
6	A	406	NAG	C2-N2-C7	2.32	126.33	122.94
6	A	405	NAG	C1-O5-C5	2.41	115.49	112.17
5	A	401	CUY	OAQ-CAP-CAO	2.74	119.89	111.90
6	A	406	NAG	C1-C2-N2	2.92	115.48	110.49
6	A	402	NAG	C1-O5-C5	3.45	116.92	112.17
10	D	308	D3D	O8-C22-C23	3.97	119.78	111.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	407	EDO	1	0
11	E	302	ACT	3	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	267/300 (89%)	0.59	17 (6%)	20 15	31, 58, 100, 204	0
2	B	97/99 (97%)	0.45	1 (1%)	82 80	35, 62, 86, 104	0
3	D	198/204 (97%)	0.26	3 (1%)	74 71	28, 50, 86, 102	0
4	E	248/249 (99%)	0.17	1 (0%)	92 91	19, 39, 78, 94	0
All	All	810/852 (95%)	0.36	22 (2%)	55 49	19, 50, 88, 204	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	LEU	3.4
1	A	204	LEU	3.2
1	A	177	GLY	2.9
4	E	187	ALA	2.9
3	D	191	ILE	2.9
1	A	109	ALA	2.9
1	A	239	ALA	2.7
1	A	202	LEU	2.7
1	A	79	ARG	2.5
1	A	251	VAL	2.5
1	A	252	ALA	2.5
1	A	169	TYR	2.4
1	A	119	GLY	2.4
1	A	144	PHE	2.3
3	D	24	HIS	2.3
1	A	110	ILE	2.1
2	B	92	PRO	2.1
3	D	145	SER	2.1
1	A	173	VAL	2.0
1	A	171	LEU	2.0
1	A	6	GLY	2.0
1	A	247	ALA	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 carbohydrates 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. 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
10	D3D	D	308	49/51	0.94	0.33	2.32	32,36,41,48	0
5	CUY	A	401	23/44	0.93	0.32	2.24	43,47,49,50	0
6	NAG	A	405	14/15	0.83	0.29	1.34	68,74,76,77	0
11	ACT	E	302	4/4	0.94	0.21	0.63	55,56,56,57	0
9	NA	E	303	1/1	0.85	0.20	0.13	62,62,62,62	0
8	EDO	D	302	4/4	0.85	0.18	-0.29	62,63,64,65	0
8	EDO	A	407	4/4	0.87	0.20	-0.36	46,46,47,47	0
8	EDO	D	305	4/4	0.88	0.17	-0.46	71,71,72,72	0
8	EDO	D	304	4/4	0.92	0.15	-0.78	61,62,63,64	0
8	EDO	D	303	4/4	0.89	0.16	-1.00	63,63,64,65	0
12	CL	E	304	1/1	0.94	0.14	-2.38	57,57,57,57	0
8	EDO	A	409	4/4	0.90	0.16	-2.38	56,57,58,59	0
9	NA	D	307	1/1	0.88	0.27	-	63,63,63,63	0
7	FUC	A	404	10/11	0.76	0.32	-	71,71,73,73	4
8	EDO	A	411	4/4	0.72	0.21	-	75,75,76,76	0
8	EDO	B	201	4/4	0.78	0.26	-	59,60,60,60	0
6	NAG	A	402	14/15	0.69	0.21	-	97,98,99,99	0
8	EDO	A	410	4/4	0.75	0.23	-	74,74,75,75	0
8	EDO	D	301	4/4	0.53	0.25	-	76,76,77,77	0
11	ACT	E	301	4/4	0.99	0.22	-	40,40,40,40	0
8	EDO	A	408	4/4	0.83	0.21	-	69,70,71,72	0
6	NAG	A	406	14/15	0.87	0.16	-	67,71,73,73	5
7	FUC	A	403	10/11	0.82	0.33	-	77,77,78,78	4
8	EDO	D	306	4/4	0.80	0.31	-	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.