



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:00 PM UTC

PDB ID : 7UVF / pdb_00007uvf
Title : Crystal structure of ZED8 Fab complex with CD8 alpha
Authors : Yu, C.; Davies, C.; Koerber, J.T.; Williams, S.
Deposited on : 2022-05-01
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

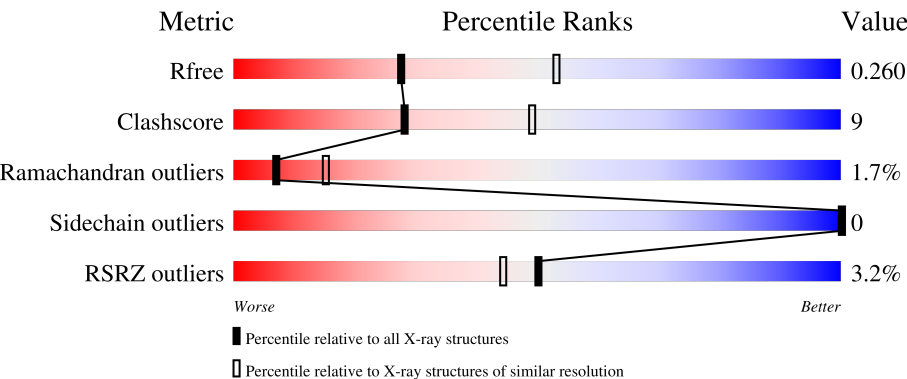
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	128	81%10%9%
1	B	128	2% 78%12%9%
2	H	221	2% 77%18%5%
2	X	221	7% 71%23%5%
3	L	214	5% 79%19%

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Mol	Chain	Length	Quality of chain
3	Y	214	76% 23%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8370 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 CD8 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	0	1	0
			935	601	159	171	4			
1	B	117	Total	C	N	O	S	0	1	0
			939	604	160	171	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	GLY	-	expression tag	UNP P01732
A	122	ASN	-	expression tag	UNP P01732
A	123	SER	-	expression tag	UNP P01732
A	124	HIS	-	expression tag	UNP P01732
A	125	HIS	-	expression tag	UNP P01732
A	126	HIS	-	expression tag	UNP P01732
A	127	HIS	-	expression tag	UNP P01732
A	128	HIS	-	expression tag	UNP P01732
B	121	GLY	-	expression tag	UNP P01732
B	122	ASN	-	expression tag	UNP P01732
B	123	SER	-	expression tag	UNP P01732
B	124	HIS	-	expression tag	UNP P01732
B	125	HIS	-	expression tag	UNP P01732
B	126	HIS	-	expression tag	UNP P01732
B	127	HIS	-	expression tag	UNP P01732
B	128	HIS	-	expression tag	UNP P01732

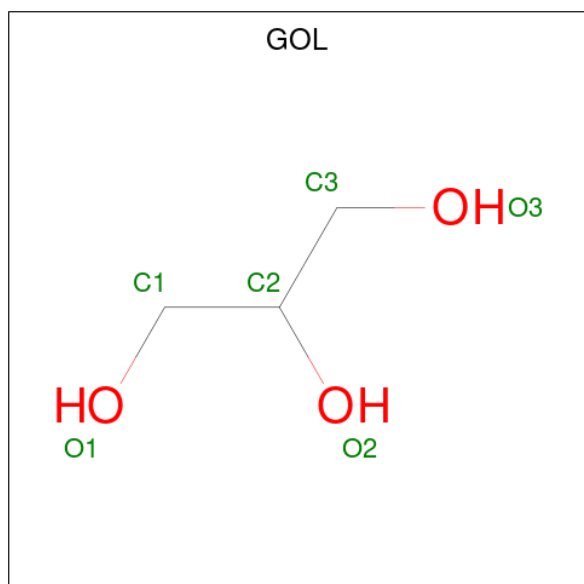
- Molecule 2 is a protein called Immunoglobulin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	210	Total	C	N	O	S	0	0	0
			1568	992	261	311	4			
2	X	210	Total	C	N	O	S	0	0	0
			1569	992	261	312	4			

- Molecule 3 is a protein called Immunoglobulin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1572	975	261	332	4			
3	Y	213	Total	C	N	O	S	0	0	0
			1607	1002	266	335	4			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Cl	0	0
			1	1		
5	X	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	44	Total	O	0	0
			44	44		
6	B	35	Total	O	0	0
			35	35		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	32	Total 32	O 32	0	0
6	L	18	Total 18	O 18	0	0
6	Y	26	Total 26	O 26	0	0
6	X	17	Total 17	O 17	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: T-cell surface glycoprotein CD8 alpha chain

Chain A: 



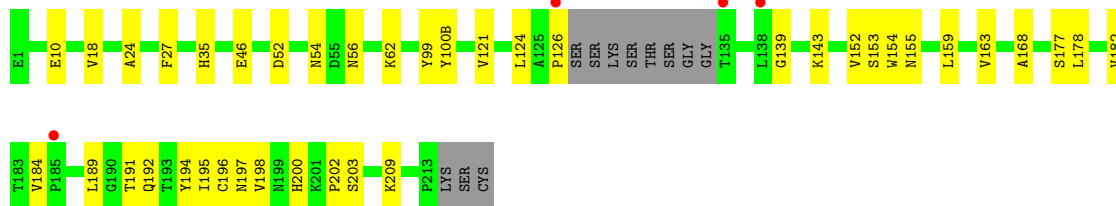
- Molecule 1: T-cell surface glycoprotein CD8 alpha chain

Chain B: 



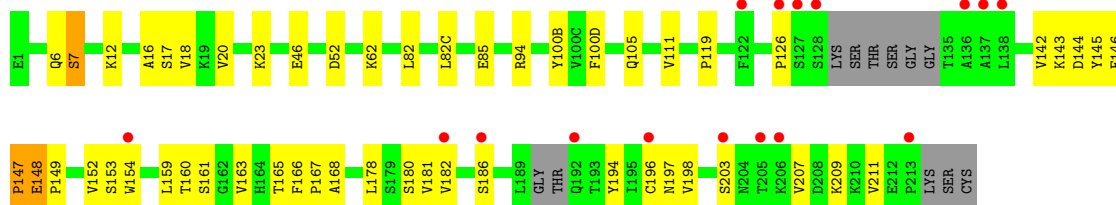
- Molecule 2: Immunoglobulin heavy chain

Chain H: 

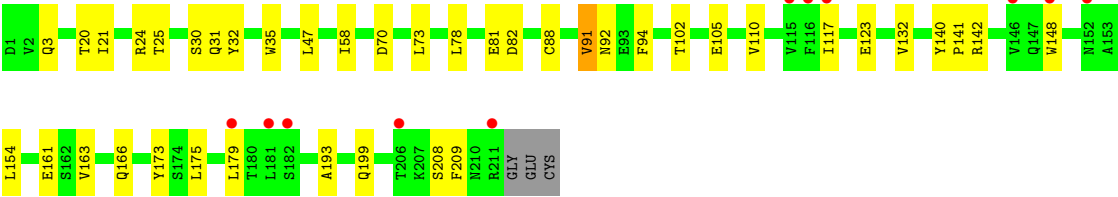
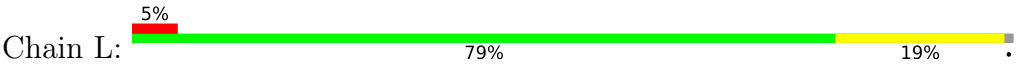


- Molecule 2: Immunoglobulin heavy chain

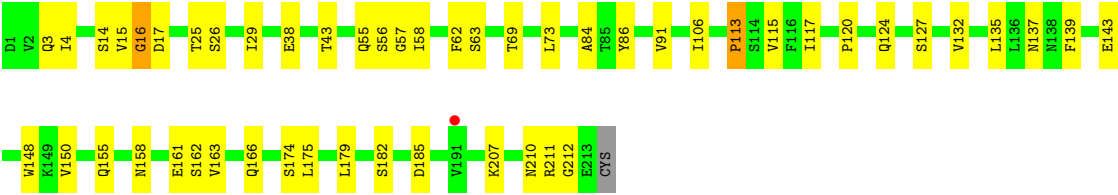
Chain X: 



- Molecule 3: Immunoglobulin light chain



● Molecule 3: Immunoglobulin light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	268.97Å 59.44Å 111.38Å 90.00° 112.29° 90.00°	Depositor
Resolution (Å)	34.35 – 2.60 34.35 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.6 (34.35-2.60) 94.7 (34.35-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.16	Depositor
R, R_{free}	0.198 , 0.259 0.198 , 0.260	Depositor DCC
R_{free} test set	2430 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8370	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: CL, GOL

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	0.44	0/962	0.62	0/1307
1	B	0.46	0/966	0.62	0/1311
2	H	0.34	0/1607	0.55	0/2198
2	X	0.36	0/1607	0.62	0/2196
3	L	0.32	0/1604	0.56	0/2189
3	Y	0.33	0/1641	0.59	0/2238
All	All	0.37	0/8387	0.59	0/11439

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	X	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	X	203	SER	Peptide

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	935	0	907	9	0
1	B	939	0	918	12	0
2	H	1568	0	1507	26	0
2	X	1569	0	1506	43	0
3	L	1572	0	1459	32	0
3	Y	1607	0	1516	36	0
4	B	6	0	8	0	0
5	H	1	0	0	1	0
5	X	1	0	0	0	0
6	A	44	0	0	1	0
6	B	35	0	0	1	0
6	H	32	0	0	0	0
6	L	18	0	0	1	0
6	X	17	0	0	0	0
6	Y	26	0	0	1	0
All	All	8370	0	7821	143	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 9.

All (143) 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:X:152:VAL:HG12	2:X:198:VAL:HG12	1.71	0.72
2:X:119:PRO:HB3	2:X:145:TYR:HB3	1.73	0.70
3:L:132:VAL:HG13	3:L:179:LEU:HB2	1.74	0.69
3:Y:163:VAL:HG22	3:Y:175:LEU:HD12	1.74	0.69
1:A:30:THR:HB	1:A:98:SER:HA	1.74	0.68
2:X:18:VAL:HG12	2:X:82(C):LEU:HD11	1.76	0.67
2:H:10:GLU:HG2	2:H:18:VAL:HG23	1.76	0.67
3:Y:4:ILE:HG12	3:Y:25:THR:HG22	1.76	0.67
3:L:21:ILE:HD13	3:L:102:THR:HB	1.78	0.65
3:Y:124:GLN:O	3:Y:127:SER:N	2.20	0.65
1:B:115:LYS:NZ	2:X:52:ASP:OD1	2.28	0.62
2:X:194:TYR:O	2:X:211:VAL:HG22	2.00	0.61
3:L:161:GLU:HG2	3:L:175:LEU:HD21	1.81	0.61
2:H:126:PRO:HG2	2:H:189:LEU:HD21	1.82	0.61
3:L:47:LEU:HD23	3:L:58:ILE:HD12	1.83	0.60
3:Y:3:GLN:HG3	3:Y:26:SER:HB3	1.82	0.60
2:X:165:THR:HG23	2:X:180:SER:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:24:ARG:HD3	3:L:70:ASP:OD1	2.03	0.59
3:Y:161:GLU:HG2	3:Y:175:LEU:HD21	1.86	0.57
3:L:163:VAL:HG22	3:L:175:LEU:HD12	1.85	0.57
2:H:200:HIS:ND1	2:H:203:SER:OG	2.21	0.57
3:Y:17:ASP:N	3:Y:17:ASP:OD1	2.36	0.57
3:Y:106:ILE:O	3:Y:166:GLN:NE2	2.35	0.57
3:Y:135:LEU:HD21	3:Y:137:ASN:HB2	1.86	0.57
3:L:117:ILE:HD13	3:L:208:SER:HA	1.86	0.57
3:L:78:LEU:HD12	3:L:82:ASP:HB2	1.86	0.57
1:A:101:ILE:HD11	1:B:58:LYS:HE3	1.87	0.57
3:Y:25:THR:HG21	3:Y:29:ILE:HD13	1.87	0.56
2:H:54:ASN:HB3	2:H:56:ASN:H	1.68	0.56
3:L:105:GLU:HB3	3:L:166:GLN:NE2	2.19	0.56
2:X:159:LEU:O	2:X:161:SER:N	2.33	0.56
2:H:163:VAL:HG22	2:H:182:VAL:HB	1.89	0.55
2:X:82:LEU:HB3	2:X:82(C):LEU:HD21	1.89	0.55
2:H:152:VAL:HG12	2:H:198:VAL:HG22	1.88	0.55
3:Y:182:SER:HB3	3:Y:185:ASP:HB2	1.89	0.54
1:A:67:ARG:HD2	1:A:83:ASP:OD1	2.08	0.54
2:H:168:ALA:HA	2:H:178:LEU:HB3	1.88	0.54
3:L:105:GLU:HB3	3:L:166:GLN:HE22	1.72	0.54
2:X:119:PRO:HB2	2:X:142:VAL:HG23	1.90	0.54
2:X:146:PHE:CD2	2:X:147:PRO:HB3	2.43	0.54
2:H:46:GLU:OE2	2:H:62:LYS:NZ	2.29	0.54
1:B:67:ARG:NH2	6:B:302:HOH:O	2.40	0.53
1:A:4:ARG:HG3	1:A:25:LEU:HD21	1.90	0.53
3:Y:143:GLU:N	3:Y:143:GLU:OE1	2.41	0.53
3:Y:3:GLN:NE2	6:Y:302:HOH:O	2.40	0.52
1:B:12:TRP:CZ3	1:B:110:VAL:HG22	2.44	0.52
2:H:209:LYS:NZ	3:L:123:GLU:OE2	2.36	0.52
2:H:100(B):TYR:HB2	3:L:91:VAL:CG2	2.40	0.52
3:Y:14:SER:O	3:Y:16:GLY:N	2.42	0.52
3:L:193:ALA:HA	3:L:208:SER:HB2	1.92	0.52
1:A:14:LEU:HB3	3:L:94:PHE:HB2	1.92	0.52
3:Y:135:LEU:CD1	2:X:181:VAL:HG21	2.40	0.52
3:Y:117:ILE:HG22	3:Y:207:LYS:HB3	1.92	0.51
3:L:166:GLN:HG3	3:L:173:TYR:CZ	2.45	0.51
1:A:4:ARG:NH2	6:A:201:HOH:O	2.27	0.51
3:Y:91:VAL:CG2	2:X:100(B):TYR:HB2	2.40	0.51
2:X:46:GLU:OE2	2:X:62:LYS:NZ	2.35	0.51
1:B:67:ARG:HD2	1:B:83:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:155:GLN:OE1	3:Y:158:ASN:ND2	2.42	0.51
2:X:7:SER:HB3	2:X:20:VAL:HG23	1.94	0.50
2:X:146:PHE:CG	2:X:147:PRO:HB3	2.46	0.50
2:H:200:HIS:CD2	2:H:202:PRO:HD2	2.47	0.50
3:Y:120:PRO:HD3	3:Y:132:VAL:HG22	1.94	0.50
2:H:191:THR:OG1	2:H:192:GLN:N	2.42	0.50
2:X:143:LYS:HE2	2:X:144:ASP:OD1	2.12	0.49
3:Y:148:TRP:CE2	3:Y:179:LEU:HB2	2.48	0.49
3:L:208:SER:OG	3:L:209:PHE:N	2.43	0.48
3:Y:62:PHE:HE1	3:Y:86:TYR:HE2	1.60	0.48
2:X:94:ARG:O	2:X:100(D):PHE:HA	2.13	0.48
3:L:140:TYR:CD1	3:L:141:PRO:HA	2.49	0.48
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.96	0.48
2:X:152:VAL:HG12	2:X:198:VAL:CG1	2.42	0.48
3:L:32:TYR:O	3:L:91:VAL:HG12	2.13	0.47
3:Y:210:ASN:O	3:Y:212:GLY:N	2.47	0.47
3:Y:135:LEU:CD2	3:Y:137:ASN:HB2	2.44	0.47
2:X:152:VAL:HG21	2:X:180:SER:CB	2.44	0.47
2:H:153:SER:OG	2:H:197:ASN:OD1	2.32	0.47
1:A:70:GLY:HA2	1:A:78:VAL:O	2.15	0.47
3:Y:115:VAL:HA	3:Y:135:LEU:O	2.14	0.47
3:Y:57:GLY:O	3:Y:58:ILE:HD12	2.16	0.46
3:Y:135:LEU:HD11	2:X:181:VAL:HG21	1.96	0.46
3:Y:150:VAL:CG1	3:Y:155:GLN:HE21	2.28	0.46
2:H:99:TYR:O	3:L:91:VAL:CG2	2.63	0.46
3:L:148:TRP:CB	3:L:179:LEU:HD21	2.45	0.46
2:X:152:VAL:HA	2:X:197:ASN:O	2.15	0.45
3:L:132:VAL:CG1	3:L:179:LEU:HB2	2.44	0.45
3:L:3:GLN:O	3:L:25:THR:HA	2.17	0.45
3:Y:63:SER:O	3:Y:73:LEU:HD12	2.16	0.45
1:A:86:ARG:HD3	6:L:304:HOH:O	2.15	0.45
2:X:152:VAL:HG21	2:X:180:SER:HB2	1.99	0.45
1:B:28:ASN:OD1	1:B:28:ASN:N	2.47	0.45
3:Y:91:VAL:HG22	2:X:100(B):TYR:HB2	1.97	0.44
2:X:153:SER:OG	2:X:154:TRP:N	2.50	0.44
2:H:24:ALA:HB1	2:H:27:PHE:CE1	2.52	0.44
2:H:143:LYS:HA	2:H:177:SER:HB2	2.00	0.44
3:L:30:SER:OG	3:L:31:GLN:N	2.51	0.44
2:X:6:GLN:H	2:X:105:GLN:HE22	1.66	0.44
2:H:155:ASN:HA	2:H:195:ILE:HG13	2.00	0.43
2:X:211:VAL:O	2:X:211:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:52:ASP:HB3	2:H:54:ASN:HB2	2.00	0.43
3:Y:43:THR:HG22	2:X:105:GLN:HA	2.00	0.43
1:A:12:TRP:O	1:A:112:LEU:HA	2.18	0.43
1:B:27:SER:O	1:B:29:PRO:HD3	2.17	0.43
2:X:82(C):LEU:HB3	2:X:111:VAL:HG21	2.00	0.43
3:Y:163:VAL:O	2:X:167:PRO:HG2	2.18	0.43
2:X:146:PHE:CE2	2:X:147:PRO:HB3	2.53	0.43
3:Y:113:PRO:CA	3:Y:139:PHE:HB3	2.49	0.43
2:H:121:VAL:O	2:H:209:LYS:HE3	2.19	0.43
2:H:154:TRP:CH2	2:H:196:CYS:HB3	2.53	0.43
2:X:23:LYS:O	2:X:23:LYS:HG3	2.18	0.43
2:X:148:GLU:HA	2:X:149:PRO:HA	1.72	0.43
2:X:85:GLU:OE2	2:X:85:GLU:N	2.46	0.43
1:B:34:SER:HB3	1:B:48:PHE:HE1	1.85	0.42
3:Y:162:SER:OG	2:X:167:PRO:O	2.37	0.42
2:X:147:PRO:O	2:X:148:GLU:HB2	2.20	0.42
3:L:81:GLU:OE1	3:L:81:GLU:N	2.43	0.42
3:L:161:GLU:OE1	3:L:175:LEU:HD11	2.18	0.42
2:X:196:CYS:N	2:X:209:LYS:O	2.32	0.42
2:H:124:LEU:O	2:H:139:GLY:N	2.53	0.42
3:Y:25:THR:OG1	3:Y:69:THR:HA	2.19	0.42
2:X:168:ALA:HA	2:X:178:LEU:HB3	2.01	0.42
1:B:102:MET:HB3	1:B:102:MET:HE2	1.81	0.42
3:L:110:VAL:HG11	3:L:199:GLN:HG2	2.02	0.42
2:X:152:VAL:CG1	2:X:198:VAL:HG12	2.46	0.42
2:X:163:VAL:HG22	2:X:182:VAL:HB	2.01	0.42
2:H:200:HIS:CE1	2:H:203:SER:HG	2.34	0.42
3:L:81:GLU:H	3:L:81:GLU:CD	2.25	0.41
2:H:184:VAL:HG11	2:H:194:TYR:CE2	2.55	0.41
3:L:32:TYR:HB2	3:L:92:ASN:HB2	2.02	0.41
1:B:64:ASP:OD2	1:B:67:ARG:N	2.51	0.41
3:L:20:THR:HA	3:L:73:LEU:O	2.20	0.41
2:H:35:HIS:NE2	5:H:301:CL:CL	2.90	0.41
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.56	0.41
3:Y:55:GLN:HG2	3:Y:56:SER:N	2.36	0.41
1:B:56:LYS:HB3	1:B:56:LYS:HE3	1.90	0.41
3:L:142:ARG:HH21	3:L:173:TYR:HE2	1.68	0.41
2:X:12:LYS:HD2	2:X:17:SER:O	2.21	0.41
1:B:48:PHE:CD2	1:B:60:ALA:HB2	2.56	0.40
3:Y:174:SER:O	2:X:166:PHE:HE2	2.04	0.40
3:Y:38:GLU:O	3:Y:84:ALA:HB1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:145:TYR:OH	2:X:148:GLU:OE2	2.29	0.40
2:H:99:TYR:O	3:L:91:VAL:HG22	2.22	0.40
2:X:146:PHE:CD1	2:X:147:PRO:HB3	2.57	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	116/128 (91%)	113 (97%)	3 (3%)	0	100	100
1	B	116/128 (91%)	104 (90%)	8 (7%)	4 (3%)	3	4
2	H	206/221 (93%)	195 (95%)	11 (5%)	0	100	100
2	X	204/221 (92%)	184 (90%)	12 (6%)	8 (4%)	2	3
3	L	209/214 (98%)	186 (89%)	21 (10%)	2 (1%)	12	28
3	Y	211/214 (99%)	193 (92%)	14 (7%)	4 (2%)	6	13
All	All	1062/1126 (94%)	975 (92%)	69 (6%)	18 (2%)	7	15

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	43	ALA
3	Y	15	VAL
2	X	147	PRO
2	X	207	VAL
3	L	154	LEU
3	Y	211	ARG
2	X	186	SER
1	B	27	SER
1	B	44	ALA

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Mol	Chain	Res	Type
3	Y	113	PRO
3	L	91	VAL
1	B	64	ASP
2	X	7	SER
2	X	16	ALA
2	X	160	THR
3	Y	16	GLY
2	X	126	PRO
2	X	148	GLU

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	103/113 (91%)	103 (100%)	0	100	100
1	B	104/113 (92%)	104 (100%)	0	100	100
2	H	172/185 (93%)	172 (100%)	0	100	100
2	X	173/185 (94%)	173 (100%)	0	100	100
3	L	176/191 (92%)	176 (100%)	0	100	100
3	Y	182/191 (95%)	182 (100%)	0	100	100
All	All	910/978 (93%)	910 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	23	GLN
3	L	37	GLN
3	L	79	GLN
3	L	124	GLN
3	L	155	GLN
3	L	210	ASN
3	Y	138	ASN

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Mol	Chain	Res	Type
3	Y	160	GLN
3	Y	199	GLN
3	Y	210	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
4	GOL	B	201	-	5,5,5	0.66	0	5,5,5	1.02	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
4	GOL	B	201	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	201	GOL	O1-C1-C2-C3
4	B	201	GOL	O1-C1-C2-O2
4	B	201	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	117/128 (91%)	-0.44	0 100 100	20, 46, 76, 107	1 (0%)
1	B	117/128 (91%)	-0.19	2 (1%) 69 64	23, 52, 94, 134	1 (0%)
2	H	210/221 (95%)	-0.03	4 (1%) 66 61	38, 70, 115, 141	0
2	X	210/221 (95%)	0.31	16 (7%) 20 16	43, 85, 128, 150	0
3	L	211/214 (98%)	0.33	11 (5%) 33 27	43, 95, 134, 161	0
3	Y	213/214 (99%)	0.21	1 (0%) 87 85	39, 92, 118, 139	0
All	All	1078/1126 (95%)	0.09	34 (3%) 50 44	20, 77, 126, 161	2 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	X	136	ALA	4.5
3	L	179	LEU	4.4
2	H	126	PRO	3.8
2	X	186	SER	3.4
3	L	146	VAL	3.0
2	X	213	PRO	2.8
2	X	196	CYS	2.8
2	H	135	THR	2.7
1	B	29	PRO	2.7
3	L	206	THR	2.7
2	X	137	ALA	2.5
3	L	152	ASN	2.5
2	X	182	VAL	2.5
2	X	206	LYS	2.4
3	L	182	SER	2.4
2	X	154	TRP	2.4
3	L	117	ILE	2.3
2	X	126	PRO	2.3
3	L	115	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	X	122	PHE	2.3
2	X	138	LEU	2.2
2	X	192	GLN	2.2
2	X	128	SER	2.2
2	X	203	SER	2.2
2	X	205	THR	2.1
3	L	116	PHE	2.1
3	L	211	ARG	2.1
3	L	181	LEU	2.1
1	B	30	THR	2.1
2	X	127	SER	2.0
3	L	148	TRP	2.0
2	H	138	LEU	2.0
3	Y	191	VAL	2.0
2	H	185	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	201	6/6	0.89	0.13	50,61,74,75	0
5	CL	H	301	1/1	0.96	0.11	64,64,64,64	0
5	CL	X	301	1/1	0.97	0.10	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.