Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:43 pm BST

PDB ID	:	3QH3
Title	:	The crystal structure of TCR A6
Authors	:	Borbulevych, O.Y.; Baker, B.M.
Deposited on	:	2011-01-25
Resolution	:	2.19 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 following versions of software and data (see references ⓘ) were used in the production of this report:

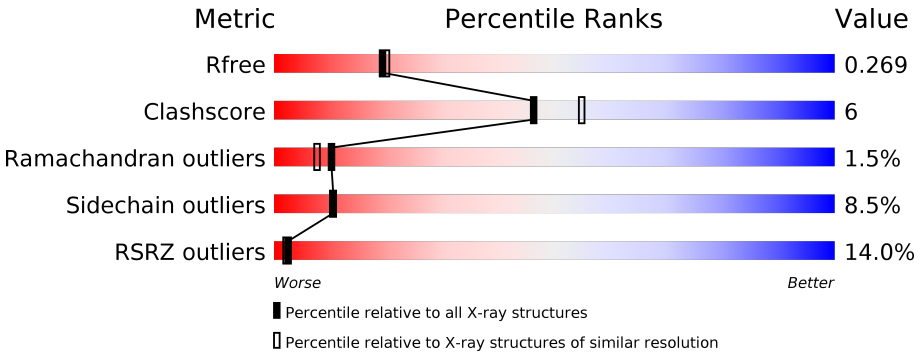
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.19 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 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 <=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	194	18% 76% 21% •
1	C	194	22% 79% 14% 6% •
2	B	245	9% 80% 18% •
2	D	245	9% 81% 16% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7190 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.

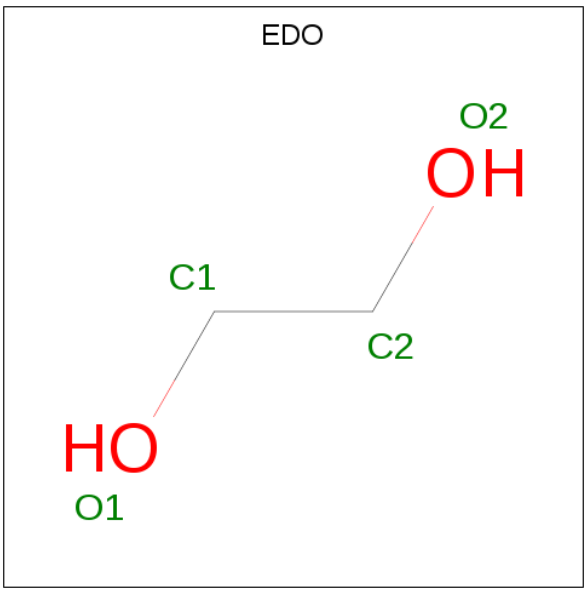
- Molecule 1 is a protein called A6 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	2	0
			1512	937	250	317	8			
1	C	194	Total	C	N	O	S	0	1	0
			1506	933	250	315	8			

- Molecule 2 is a protein called A6 beta chain.

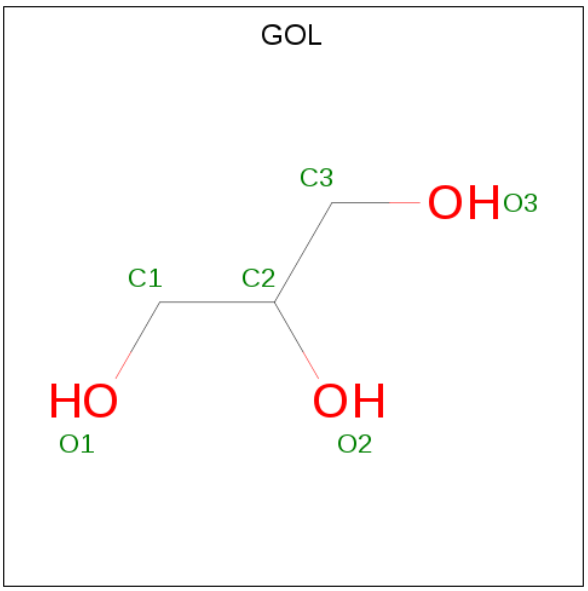
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	245	Total	C	N	O	S	0	0	0
			1928	1209	338	372	9			
2	D	241	Total	C	N	O	S	0	3	0
			1918	1208	331	369	10			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

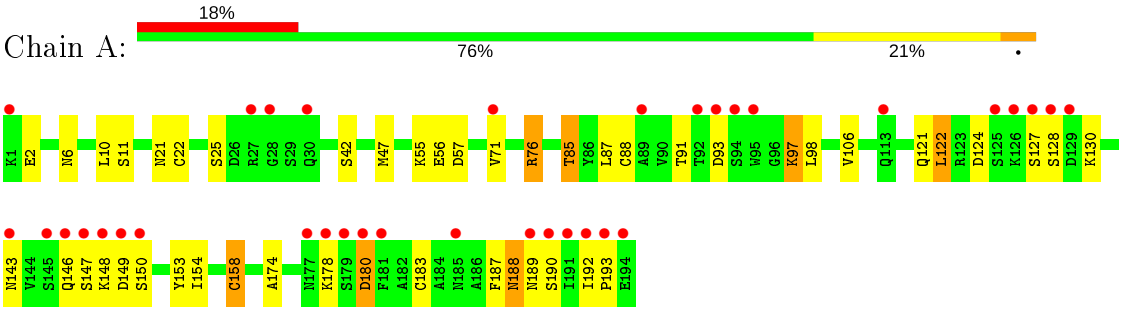
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	52	Total O 52 52	0	0
5	B	63	Total O 63 63	0	0
5	C	51	Total O 51 51	0	0
5	D	90	Total O 90 90	0	0

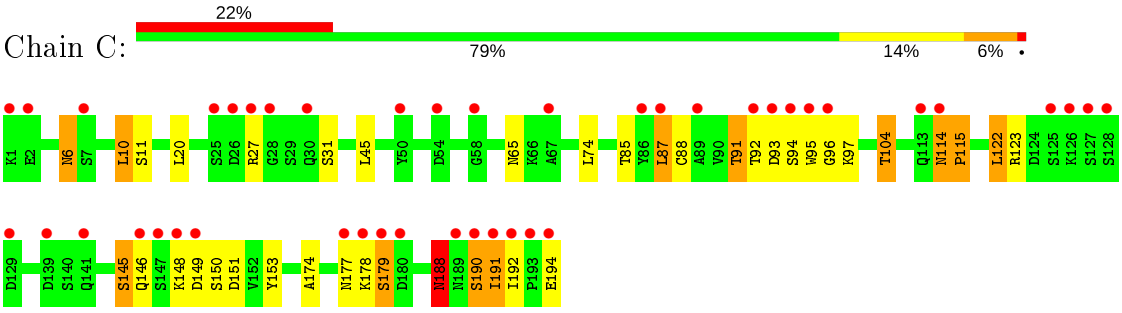
3 Residue-property plots (i)

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.

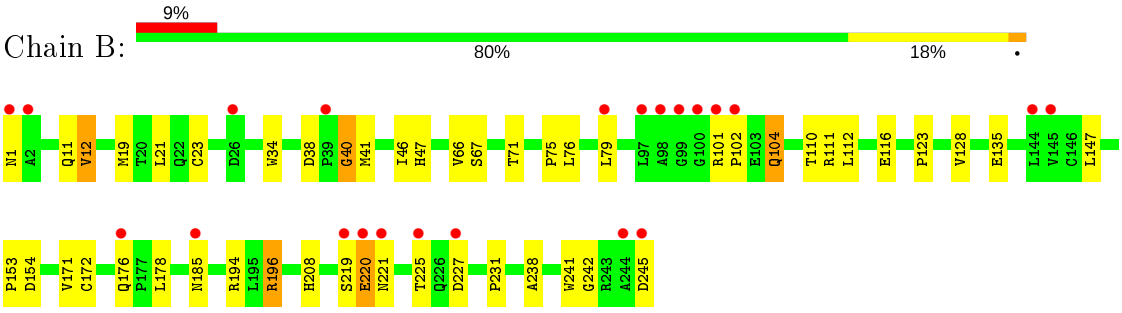
- Molecule 1: A6 alpha chain



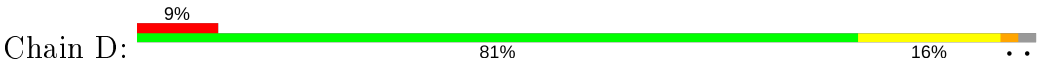
- Molecule 1: A6 alpha chain

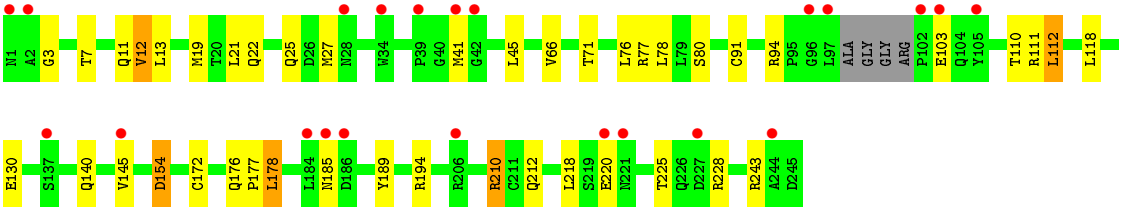


- Molecule 2: A6 beta chain



- Molecule 2: A6 beta chain




N1
A2
G3
T7
Q11
V12
L13
M19
T20
L21
Q22
Q25
D26
M27
N28
W34
P39
G40
M41
G42
L45
V66
T71
L76
R77
L78
L79
S80
C91
R94
P95
G96
L97
ALA
GLY
GLY
ARG
P102
E103
Q104
Y105
T110
R111
L112
L118
E130
S137
Q140
V145
D154
C172
Q176
P177
L178
L184
N185
D186
Y189
R194
R206
R210
C211
Q212
L218
S219
E220
N221
T225
Q226
D227
R228
R243
A244
D245

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.25Å 51.73Å 96.34Å 90.00° 105.05° 90.00°	Depositor
Resolution (Å)	19.86 – 2.19 19.86 – 2.19	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.86-2.19) 98.7 (19.86-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.202 , 0.274 0.197 , 0.269	Depositor DCC
R_{free} test set	2254 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	37.0	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7190	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3372e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.93	3/1548 (0.2%)	0.93	4/2098 (0.2%)
1	C	0.84	2/1539 (0.1%)	0.87	1/2086 (0.0%)
2	B	0.85	1/1981 (0.1%)	0.87	1/2699 (0.0%)
2	D	0.97	1/1979 (0.1%)	0.97	5/2695 (0.2%)
All	All	0.90	7/7047 (0.1%)	0.91	11/9578 (0.1%)

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
1	C	0	4
2	B	0	1
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	CYS	CB-SG	-7.02	1.70	1.82
1	A	88	CYS	CB-SG	-6.70	1.70	1.82
2	B	172	CYS	CB-SG	-6.20	1.71	1.82
1	C	88	CYS	CB-SG	-5.48	1.72	1.81
2	D	91	CYS	CB-SG	-5.46	1.73	1.81
1	A	106	VAL	CB-CG2	5.24	1.63	1.52
1	C	93	ASP	CG-OD2	5.08	1.37	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	158	CYS	CA-CB-SG	9.09	130.36	114.00
2	D	210	ARG	NE-CZ-NH2	-8.87	115.86	120.30
2	D	178	LEU	CA-CB-CG	7.88	133.42	115.30
1	A	87	LEU	CA-CB-CG	6.70	130.71	115.30
1	C	122	LEU	CA-CB-CG	6.68	130.66	115.30
1	A	122	LEU	CA-CB-CG	6.20	129.56	115.30
2	D	112	LEU	CA-CB-CG	5.63	128.25	115.30
2	D	145	VAL	CG1-CB-CG2	5.57	119.81	110.90
2	D	12	VAL	CB-CA-C	-5.46	101.02	111.40
1	A	76	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	B	196	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	171	VAL	Peptide
1	C	115	PRO	Peptide
1	C	188	ASN	Peptide
1	C	91	THR	Peptide
1	C	96	GLY	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	1512	0	1429	17	0
1	C	1506	0	1423	24	0
2	B	1928	0	1829	18	0
2	D	1918	0	1832	32	0
3	A	12	0	18	2	0
3	B	12	0	18	0	0
3	C	8	0	12	1	0
3	D	8	0	12	3	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	52	0	0	1	0
5	B	63	0	0	0	0
5	C	51	0	0	2	0
5	D	90	0	0	1	0
All	All	7190	0	6613	85	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 6.

All (85) 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:D:19[A]:MET:HE2	2:D:21[A]:LEU:HD23	1.50	0.92
2:D:19[A]:MET:CE	2:D:21[A]:LEU:HD23	2.01	0.89
2:D:19[A]:MET:CE	2:D:21[A]:LEU:CD2	2.53	0.87
2:D:228:ARG:HE	3:D:249:EDO:H11	1.43	0.83
2:D:3:GLY:HA2	2:D:27:MET:CE	2.11	0.81
2:D:220:GLU:HG3	5:D:280:HOH:O	1.81	0.80
2:D:19[A]:MET:HE2	2:D:21[A]:LEU:CD2	2.11	0.80
2:B:12:VAL:HG13	2:B:153:PRO:HG3	1.65	0.78
1:C:97:LYS:HE3	2:D:45:LEU:HD23	1.66	0.78
2:D:19[A]:MET:HE1	2:D:21[A]:LEU:CD2	2.13	0.76
1:C:6[B]:ASN:HB3	1:C:104:THR:HG21	1.72	0.71
2:D:3:GLY:HA2	2:D:27:MET:HE1	1.73	0.69
1:A:143:ASN:O	1:A:190:SER:HB2	1.92	0.69
1:C:123:ARG:HB2	3:C:197:EDO:H11	1.74	0.69
2:D:19[A]:MET:HE1	2:D:21[A]:LEU:HD21	1.74	0.68
2:D:19[A]:MET:CE	2:D:21[A]:LEU:HD21	2.24	0.67
2:D:3:GLY:HA2	2:D:27:MET:HE3	1.78	0.66
1:A:93:ASP:HB2	1:A:97:LYS:H	1.62	0.65
1:A:85:THR:HG23	5:A:210:HOH:O	1.98	0.64
1:C:31:SER:HB2	1:C:91:THR:CG2	2.30	0.61
1:C:95:TRP:HB3	2:D:94:ARG:HH22	1.66	0.60
1:C:6[A]:ASN:HB3	1:C:104:THR:HG21	1.82	0.60
1:C:45:LEU:HD23	2:D:103:GLU:HB3	1.85	0.58
2:B:38:ASP:O	2:B:40:GLY:N	2.35	0.57
2:B:101:ARG:HD3	2:B:102:PRO:HD2	1.86	0.57
1:A:187:PHE:O	1:A:189:ASN:N	2.38	0.56
1:A:147:SER:H	1:A:154:ILE:HD12	1.72	0.55
2:B:219:SER:O	2:B:221:ASN:N	2.40	0.54
2:D:13:LEU:HD21	2:D:19[B]:MET:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:GLU:HB3	1:A:25:SER:HB3	1.91	0.53
1:A:121:GLN:HG3	1:A:183:CYS:SG	2.50	0.52
1:C:146:GLN:NE2	2:D:178:LEU:HD11	2.25	0.52
2:B:11:GLN:HB3	2:B:112:LEU:HD13	1.91	0.52
1:C:95:TRP:HD1	2:D:94:ARG:HH12	1.57	0.52
2:B:111:ARG:NH2	2:B:154:ASP:OD1	2.44	0.51
2:D:11:GLN:HG2	2:D:19[A]:MET:SD	2.52	0.50
1:C:188:ASN:HA	1:C:191:ILE:HA	1.92	0.50
2:B:21:LEU:HD22	2:B:110:THR:HG21	1.93	0.49
2:D:78:LEU:HD12	2:D:78:LEU:N	2.27	0.49
1:A:147:SER:H	1:A:154:ILE:CD1	2.24	0.49
2:D:21[A]:LEU:HD22	2:D:110:THR:HG21	1.93	0.49
2:B:135:GLU:OE2	2:B:196:ARG:NH2	2.43	0.49
1:C:149:ASP:C	1:C:151:ASP:H	2.16	0.48
2:D:19[A]:MET:HE1	2:D:21[A]:LEU:HD23	1.85	0.48
1:A:6[B]:ASN:HD21	1:A:21:ASN:H	1.62	0.47
2:D:130:GLU:OE1	2:D:243:ARG:NH1	2.48	0.47
2:D:22:GLN:HE22	3:D:248:EDO:H11	1.79	0.47
2:B:123:PRO:HD3	2:B:231:PRO:HB3	1.97	0.47
1:C:145:SER:H	1:C:190:SER:HB3	1.79	0.47
1:C:94:SER:HB2	1:C:95:TRP:CE3	2.49	0.47
2:B:219:SER:OG	2:B:220:GLU:N	2.46	0.46
2:D:111:ARG:NH2	2:D:154:ASP:OD1	2.48	0.46
2:D:154:ASP:HB3	2:D:189:TYR:CD1	2.51	0.46
1:A:47:MET:SD	1:A:57:ASP:HB3	2.57	0.45
2:D:210:ARG:NH2	2:D:212:GLN:OE1	2.47	0.45
2:B:128:VAL:HG23	2:B:238:ALA:HB3	1.99	0.44
1:C:149:ASP:O	1:C:151:ASP:N	2.50	0.44
1:C:178:LYS:HG3	5:C:199:HOH:O	2.17	0.44
2:D:13:LEU:HD12	2:D:112:LEU:HD11	1.99	0.44
1:C:20:LEU:HD23	1:C:104:THR:HG23	2.00	0.44
2:D:118:LEU:HD22	2:D:218:LEU:HD21	1.99	0.44
2:B:147:LEU:HD23	2:B:147:LEU:HA	1.73	0.43
2:B:46:ILE:HG22	2:B:47:HIS:CD2	2.53	0.43
2:D:228:ARG:NE	3:D:249:EDO:H11	2.22	0.43
1:C:178:LYS:O	1:C:179:SER:CB	2.67	0.43
1:A:56:GLU:HG3	1:A:76:ARG:HH22	1.83	0.43
1:A:55:LYS:HD2	3:A:197:EDO:H22	2.01	0.42
2:D:21[A]:LEU:HD12	2:D:76:LEU:HD23	2.01	0.42
1:C:114:ASN:HA	1:C:115:PRO:HD3	1.73	0.42
2:B:67:SER:O	2:B:75:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:TYR:O	1:C:174:ALA:HA	2.20	0.41
1:C:6[B]:ASN:ND2	1:C:10:LEU:HD21	2.36	0.41
1:A:124:ASP:HB2	1:A:130:LYS:HB2	2.03	0.41
2:B:23:CYS:HB2	2:B:34:TRP:CZ2	2.55	0.41
2:B:21:LEU:HD12	2:B:76:LEU:HD23	2.02	0.41
1:A:153:TYR:O	1:A:174:ALA:HA	2.21	0.41
1:C:87:LEU:HD22	1:C:87:LEU:N	2.36	0.41
3:A:196:EDO:H12	2:B:104:GLN:O	2.21	0.40
1:A:6[B]:ASN:ND2	1:A:21:ASN:OD1	2.54	0.40
1:A:149:ASP:OD1	1:A:150:SER:N	2.55	0.40
1:A:21:ASN:OD1	2:D:210:ARG:NH2	2.54	0.40
1:C:104:THR:CG2	5:C:207:HOH:O	2.69	0.40
2:B:208:HIS:HB2	2:B:241:TRP:CZ3	2.57	0.40
1:C:149:ASP:C	1:C:151:ASP:N	2.74	0.40
1:C:178:LYS:HD3	1:C:178:LYS:HA	1.98	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	194/194 (100%)	175 (90%)	12 (6%)	7 (4%)	3 1
1	C	193/194 (100%)	172 (89%)	17 (9%)	4 (2%)	7 4
2	B	243/245 (99%)	233 (96%)	7 (3%)	3 (1%)	13 10
2	D	240/245 (98%)	234 (98%)	6 (2%)	0	100 100
All	All	870/878 (99%)	814 (94%)	42 (5%)	14 (2%)	10 7

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
2	B	220	GLU
1	A	146	GLN
1	A	148	LYS
1	A	180	ASP
1	C	6[A]	ASN
1	C	6[B]	ASN
1	C	150	SER
1	C	179	SER
1	A	178	LYS
1	A	192	ILE
1	A	193	PRO
2	B	40	GLY
2	B	242	GLY

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	174/172 (101%)	160 (92%)	14 (8%)	12 12
1	C	173/172 (101%)	154 (89%)	19 (11%)	6 5
2	B	209/209 (100%)	193 (92%)	16 (8%)	13 13
2	D	211/209 (101%)	194 (92%)	17 (8%)	11 12
All	All	767/762 (101%)	701 (91%)	66 (9%)	10 10

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

Mol	Chain	Res	Type
1	A	10	LEU
1	A	11	SER
1	A	42	SER
1	A	71	VAL
1	A	85	THR
1	A	91	THR
1	A	97	LYS
1	A	98	LEU

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Mol	Chain	Res	Type
1	A	122	LEU
1	A	127	SER
1	A	128	SER
1	A	158	CYS
1	A	180	ASP
1	A	188	ASN
2	B	1	ASN
2	B	12	VAL
2	B	19	MET
2	B	41	MET
2	B	66	VAL
2	B	71	THR
2	B	79	LEU
2	B	104	GLN
2	B	116	GLU
2	B	176	GLN
2	B	178	LEU
2	B	185	ASN
2	B	194	ARG
2	B	225	THR
2	B	227	ASP
2	B	245	ASP
1	C	10	LEU
1	C	11	SER
1	C	27	ARG
1	C	65	ASN
1	C	74	LEU
1	C	85	THR
1	C	87	LEU
1	C	92	THR
1	C	104	THR
1	C	114	ASN
1	C	122	LEU
1	C	145	SER
1	C	148	LYS
1	C	177	ASN
1	C	188	ASN
1	C	190	SER
1	C	191	ILE
1	C	192	ILE
1	C	194	GLU
2	D	7	THR

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Mol	Chain	Res	Type
2	D	12	VAL
2	D	25	GLN
2	D	41	MET
2	D	66	VAL
2	D	71[A]	THR
2	D	71[B]	THR
2	D	77	ARG
2	D	80	SER
2	D	140	GLN
2	D	154	ASP
2	D	172	CYS
2	D	176	GLN
2	D	177	PRO
2	D	185	ASN
2	D	194	ARG
2	D	225	THR

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

Mol	Chain	Res	Type
1	A	113	GLN
1	A	188	ASN
2	B	104	GLN
2	B	185	ASN
1	C	105	GLN
1	C	114	ASN
1	C	146	GLN
1	C	188	ASN
2	D	185	ASN
2	D	226	GLN

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)

15 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	$\#\|Z\| > 2$
3	EDO	B	249	-	3,3,3	0.80	0	2,2,2	0.46	0
3	EDO	A	197	-	3,3,3	0.49	0	2,2,2	0.85	0
3	EDO	C	197	-	3,3,3	0.76	0	2,2,2	0.36	0
3	EDO	B	247	-	3,3,3	0.37	0	2,2,2	0.55	0
4	GOL	B	246	-	5,5,5	0.70	0	5,5,5	1.65	2 (40%)
4	GOL	D	246	-	5,5,5	0.28	0	5,5,5	0.49	0
3	EDO	A	196	-	3,3,3	0.49	0	2,2,2	0.63	0
3	EDO	C	195	-	3,3,3	0.57	0	2,2,2	0.19	0
4	GOL	C	196	-	5,5,5	0.44	0	5,5,5	0.40	0
3	EDO	A	195	-	3,3,3	0.45	0	2,2,2	0.66	0
4	GOL	D	247	-	5,5,5	0.46	0	5,5,5	0.29	0
3	EDO	B	248	-	3,3,3	0.55	0	2,2,2	0.41	0
4	GOL	A	198	-	5,5,5	0.33	0	5,5,5	0.47	0
3	EDO	D	248	-	3,3,3	0.66	0	2,2,2	0.23	0
3	EDO	D	249	-	3,3,3	0.55	0	2,2,2	0.59	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
3	EDO	B	249	-	-	1/1/1/1	-
3	EDO	A	197	-	-	0/1/1/1	-
3	EDO	C	197	-	-	1/1/1/1	-
3	EDO	B	247	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	246	-	-	2/4/4/4	-
4	GOL	D	246	-	-	0/4/4/4	-
3	EDO	A	196	-	-	0/1/1/1	-
3	EDO	C	195	-	-	0/1/1/1	-
4	GOL	C	196	-	-	0/4/4/4	-
3	EDO	A	195	-	-	0/1/1/1	-
4	GOL	D	247	-	-	2/4/4/4	-
3	EDO	B	248	-	-	0/1/1/1	-
4	GOL	A	198	-	-	0/4/4/4	-
3	EDO	D	248	-	-	1/1/1/1	-
3	EDO	D	249	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	246	GOL	O3-C3-C2	-2.98	95.93	110.20
4	B	246	GOL	O2-C2-C3	-2.07	99.99	109.12

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	246	GOL	C1-C2-C3-O3
4	D	247	GOL	O1-C1-C2-C3
3	B	249	EDO	O1-C1-C2-O2
3	C	197	EDO	O1-C1-C2-O2
3	B	247	EDO	O1-C1-C2-O2
3	D	249	EDO	O1-C1-C2-O2
3	D	248	EDO	O1-C1-C2-O2
4	B	246	GOL	O2-C2-C3-O3
4	D	247	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	197	EDO	1	0
3	C	197	EDO	1	0
3	A	196	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	248	EDO	1	0
3	D	249	EDO	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	194/194 (100%)	0.99	35 (18%)	1 1	19, 38, 100, 113	0
1	C	194/194 (100%)	1.28	43 (22%)	0 0	25, 50, 97, 118	0
2	B	245/245 (100%)	0.58	22 (8%)	9 8	23, 40, 74, 88	0
2	D	241/245 (98%)	0.38	22 (9%)	9 8	17, 32, 55, 81	0
All	All	874/878 (99%)	0.77	122 (13%)	2 2	17, 38, 87, 118	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	ILE	12.7
1	A	191	ILE	11.7
1	C	193	PRO	11.5
1	C	147	SER	10.7
1	C	191	ILE	9.2
1	A	129	ASP	9.0
2	B	98	ALA	8.3
2	B	99	GLY	8.1
1	C	1	LYS	8.1
2	B	1	ASN	7.7
1	A	128	SER	7.6
1	C	192	ILE	7.4
1	C	190	SER	7.0
1	A	179	SER	6.9
1	A	190	SER	6.9
2	B	221	ASN	6.6
2	B	100	GLY	6.4
1	C	95	TRP	6.4
1	A	127	SER	6.3
1	A	180	ASP	6.3
2	B	2	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
2	B	220	GLU	6.2
1	A	193	PRO	6.1
1	C	189	ASN	6.0
1	C	177	ASN	6.0
1	C	194	GLU	5.8
1	C	27	ARG	5.5
1	A	189	ASN	5.4
1	A	147	SER	5.2
2	D	1	ASN	5.1
1	A	149	ASP	5.0
2	D	97	LEU	4.9
1	C	94	SER	4.8
2	B	245	ASP	4.8
1	A	181	PHE	4.8
1	A	178	LYS	4.5
1	A	148	LYS	4.4
1	C	128	SER	4.4
1	A	150	SER	4.3
1	C	25	SER	4.1
1	C	148	LYS	4.0
1	C	129	ASP	3.9
2	D	102	PRO	3.9
1	A	95	TRP	3.9
1	A	92	THR	3.8
1	A	185	ASN	3.8
1	A	1	LYS	3.7
1	C	92	THR	3.7
2	B	101	ARG	3.7
1	A	94	SER	3.6
2	B	227	ASP	3.5
1	C	127	SER	3.5
2	D	2	ALA	3.5
2	D	39	PRO	3.4
1	C	93	ASP	3.4
1	C	180	ASP	3.4
1	C	126	LYS	3.3
1	C	125	SER	3.3
2	B	219	SER	3.3
1	A	30	GLN	3.3
2	B	102	PRO	3.3
1	A	194	GLU	3.3
2	B	225	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	30	GLN	3.1
1	C	113	GLN	3.1
2	D	42	GLY	3.0
2	B	39	PRO	3.0
2	D	220	GLU	3.0
2	B	79	LEU	3.0
1	C	96	GLY	3.0
2	D	137	SER	2.9
1	A	27	ARG	2.8
1	C	149	ASP	2.8
1	C	50	TYR	2.7
2	D	103	GLU	2.7
1	C	179	SER	2.7
1	A	145	SER	2.7
1	C	26	ASP	2.6
1	C	58	GLY	2.6
2	B	244	ALA	2.5
1	C	87	LEU	2.5
2	B	97	LEU	2.5
1	A	177	ASN	2.5
1	C	139	ASP	2.5
2	B	185	ASN	2.5
2	D	244	ALA	2.4
1	A	113	GLN	2.4
1	C	141	GLN	2.4
2	B	144	LEU	2.4
1	C	178	LYS	2.4
2	D	28	ASN	2.4
2	D	221	ASN	2.3
1	C	2	GLU	2.3
2	B	176	GLN	2.3
1	A	89	ALA	2.3
1	C	54	ASP	2.3
1	C	89	ALA	2.2
2	B	145	VAL	2.2
2	D	206	ARG	2.2
1	C	67	ALA	2.2
2	D	186	ASP	2.2
1	C	86	TYR	2.2
2	B	26	ASP	2.2
1	C	114	ASN	2.2
1	A	143	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	7	SER	2.2
2	D	184	LEU	2.1
1	A	126	LYS	2.1
1	A	71	VAL	2.1
2	D	96	GLY	2.1
1	A	93	ASP	2.1
2	D	34	TRP	2.1
2	D	105	TYR	2.1
1	A	125	SER	2.0
2	D	227	ASP	2.0
1	A	146	GLN	2.0
2	D	145	VAL	2.0
1	A	28	GLY	2.0
1	C	28	GLY	2.0
1	C	146	GLN	2.0
2	D	185	ASN	2.0
2	D	41	MET	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. The B-factors column lists the minimum, median, 95^{th} 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(Å^2)	Q<0.9
4	GOL	A	198	6/6	0.54	0.28	52,61,63,65	0
3	EDO	C	195	4/4	0.64	0.24	58,61,62,62	0
3	EDO	B	249	4/4	0.68	0.37	40,41,42,45	0
4	GOL	C	196	6/6	0.73	0.17	66,68,69,69	0
3	EDO	D	248	4/4	0.73	0.30	50,55,56,56	0
3	EDO	A	197	4/4	0.78	0.15	48,53,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	D	249	4/4	0.82	0.17	48,49,49,50	0
3	EDO	A	196	4/4	0.83	0.62	42,45,47,50	0
3	EDO	A	195	4/4	0.83	0.18	56,60,61,61	0
3	EDO	B	248	4/4	0.83	0.34	39,46,47,49	0
3	EDO	B	247	4/4	0.87	0.21	55,56,57,57	0
4	GOL	D	246	6/6	0.87	0.16	55,56,58,58	0
4	GOL	B	246	6/6	0.88	0.18	39,43,45,48	0
3	EDO	C	197	4/4	0.91	0.20	34,40,42,50	0
4	GOL	D	247	6/6	0.92	0.17	46,49,54,56	0

6.5 Other polymers (i)

There are no such residues in this entry.