Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 08:22 PM EDT

PDB ID	:	6SRV
Title	:	Structure of the arginase-2-inhibitory human antigen-binding fragment Fab C0021144
Authors	:	Burschowsky, D.; Addyman, A.; Fiedler, S.; Groves, M.; Haynes, S.; Seewooruthun, C.; Carr, M.
Deposited on	:	2019-09-06
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

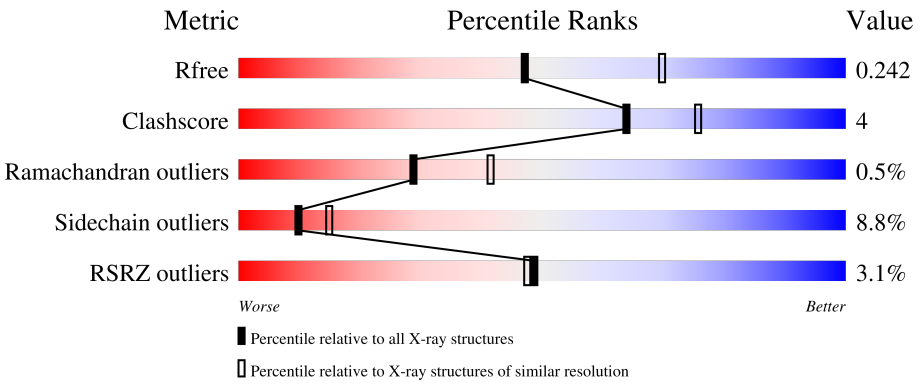
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 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 <=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	HHH	233	% 81% 13% • •
1	III	233	2% 77% 18% • •
2	LLL	220	5% 82% 13% • •
2	MMM	220	5% 81% 15% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	MMM	302	-	-	-	X
6	TRS	HHH	314	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13237 atoms, of which 6544 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 Fab C0021144 heavy chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	HHH	224	3321	1052	1647	287	328	7	94	0	0
1	III	223	3309	1048	1643	286	325	7	94	0	0

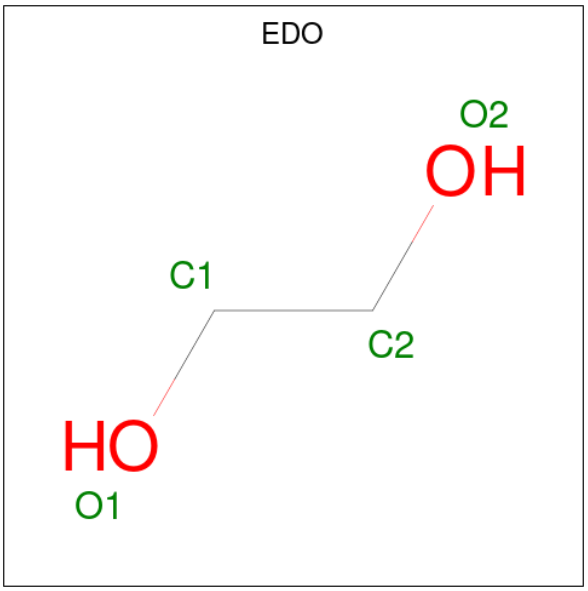
- Molecule 2 is a protein called Fab C0021144 light chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	LLL	214	3118	988	1539	261	326	4	105	0	0
2	MMM	213	3103	983	1533	260	323	4	105	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

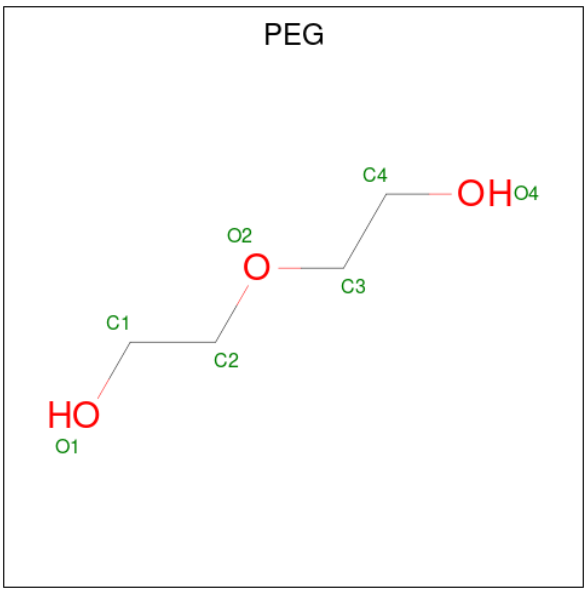
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	HHH	1	1	1	0	0
3	III	2	2	2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



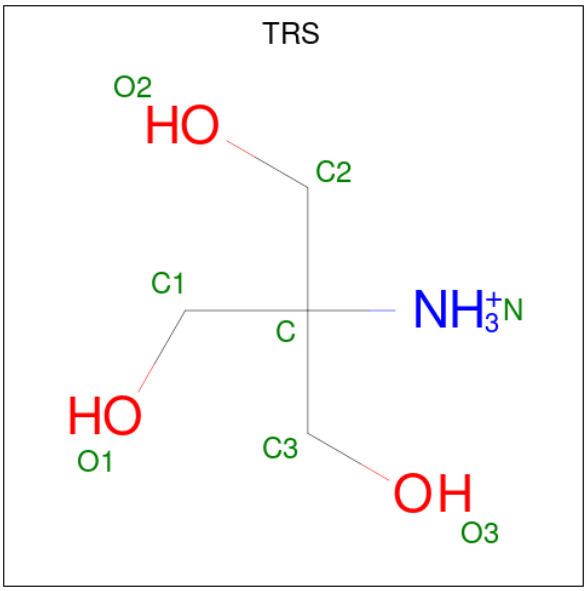
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	HHH	1	10	2	6	2	1	0
4	HHH	1	10	2	6	2	1	0
4	HHH	1	10	2	6	2	1	0
4	HHH	1	10	2	6	2	1	0
4	HHH	1	10	2	6	2	1	0
4	HHH	1	10	2	6	2	1	0
4	HHH	1	10	2	6	2	1	0
4	HHH	1	10	2	6	2	1	0
4	HHH	1	10	2	6	2	1	0
4	III	1	10	2	6	2	1	0
4	MMM	1	10	2	6	2	1	0
4	MMM	1	10	2	6	2	1	0
4	MMM	1	10	2	6	2	1	0
4	MMM	1	10	2	6	2	1	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	HHH	1	Total	C	H	O	1	0
			17	4	10	3		
5	HHH	1	Total	C	H	O	1	0
			17	4	10	3		
5	III	1	Total	C	H	O	1	0
			17	4	10	3		
5	III	1	Total	C	H	O	1	0
			17	4	10	3		
5	III	1	Total	C	H	O	1	0
			17	4	10	3		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
6	HHH	1	20	4	12	1	3	2	0
			Total	C	H	N	O		
6	HHH	1	20	4	12	1	3	2	0
			Total	C	H	N	O		
6	LLL	1	20	4	12	1	3	2	0
			Total	C	H	N	O		
6	MMM	1	20	4	12	1	3	2	0

- Molecule 7 is water.

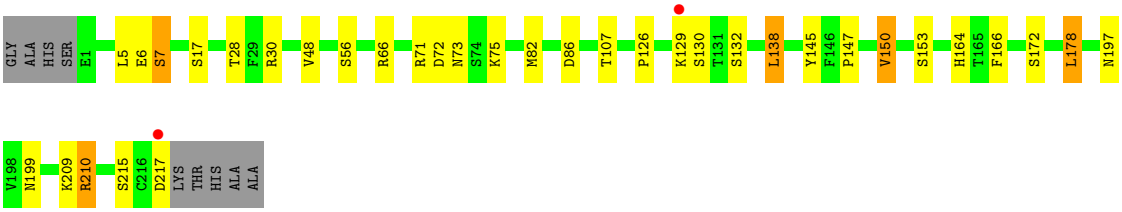
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	HHH	20	20	20	0	0
			Total	O		
7	III	23	23	23	0	0
			Total	O		
7	LLL	21	21	21	0	0
			Total	O		
7	MMM	14	14	14	0	0

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.

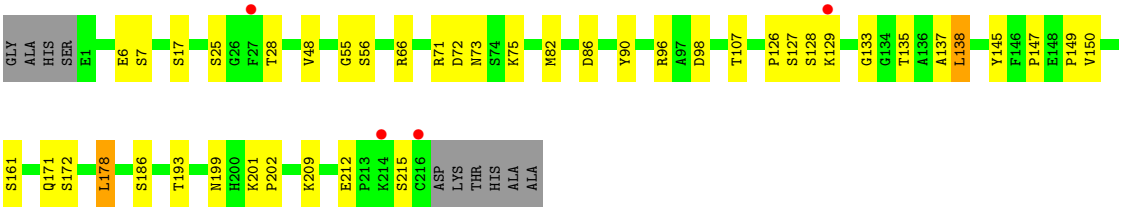
• Molecule 1: Fab C0021144 heavy chain (IgG1)

Chain HHH:



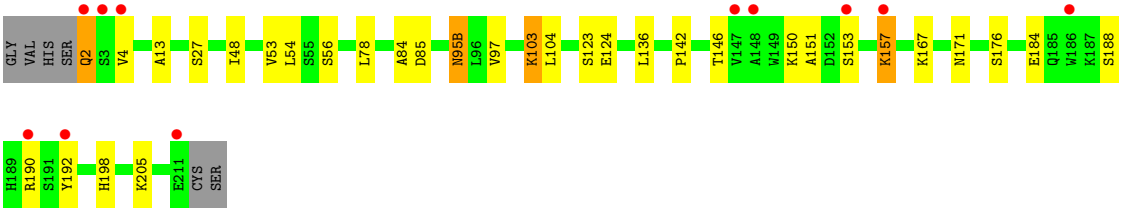
• Molecule 1: Fab C0021144 heavy chain (IgG1)

Chain III:



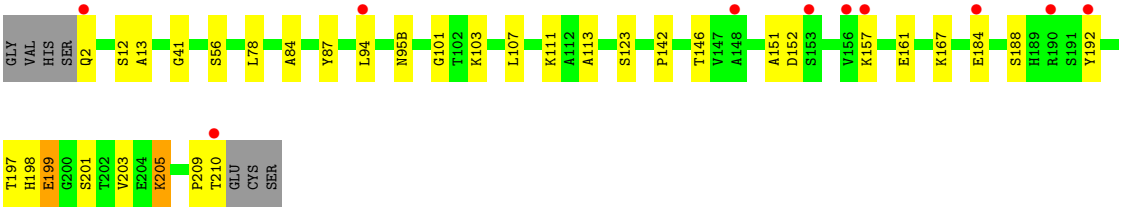
• Molecule 2: Fab C0021144 light chain (IgG1)

Chain LLL:



• Molecule 2: Fab C0021144 light chain (IgG1)

Chain MMM:


GLY
VAL
HIS
SER
Q2
S12
A13
G41
S56
L78
A84
Y87
L94
N95B
G101
T102
K103
L107
K111
A112
A113
S123
P142
T146
V147
A148
A151
D152
S153
V156
K157
E161
K167
E184
S188
H189
R190
S191
Y192
T197
H198
E199
G200
S201
T202
V203
E204
K205
P209
T210
GLU
CYS
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	172.69Å 172.69Å 211.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.90 – 2.40 49.85 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.90-2.40) 100.0 (49.85-2.40)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.205 , 0.241 0.211 , 0.242	Depositor DCC
R_{free} test set	2368 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.000 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.000 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13237	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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

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	HHH	0.78	0/1712	1.00	0/2329
1	III	0.75	0/1704	1.00	0/2318
2	LLL	0.76	0/1617	0.92	0/2213
2	MMM	0.78	0/1608	0.93	1/2201 (0.0%)
All	All	0.77	0/6641	0.97	1/9061 (0.0%)

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	HHH	0	1
1	III	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	MMM	152	ASP	CB-CA-C	5.01	120.42	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	HHH	7	SER	Peptide
1	III	133	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	HHH	1674	1647	1646	15	0
1	III	1666	1643	1642	15	0
2	LLL	1579	1539	1534	14	0
2	MMM	1570	1533	1528	14	0
3	HHH	1	0	0	0	0
3	III	2	0	0	0	0
4	HHH	36	54	54	0	0
4	III	4	6	6	0	0
4	MMM	16	24	24	1	0
5	HHH	14	20	20	0	0
5	III	21	30	30	1	0
6	HHH	16	24	24	1	0
6	LLL	8	12	12	0	0
6	MMM	8	12	12	1	0
7	HHH	20	0	0	1	0
7	III	23	0	0	1	0
7	LLL	21	0	0	1	0
7	MMM	14	0	0	0	0
All	All	6693	6544	6532	55	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 (55) 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:III:178:LEU:C	1:III:178:LEU:HD12	2.13	0.69
1:HHH:178:LEU:C	1:HHH:178:LEU:HD12	2.15	0.66
2:LLL:48:ILE:HG12	2:LLL:54:LEU:HD23	1.83	0.60
2:MMM:142:PRO:O	2:MMM:198:HIS:HE1	1.85	0.60
2:LLL:142:PRO:O	2:LLL:198:HIS:HE1	1.87	0.57
2:LLL:124:GLU:HG3	7:LLL:420:HOH:O	2.04	0.56
1:HHH:5:LEU:HD12	1:III:135:THR:HG22	1.88	0.55
1:HHH:126:PRO:HD3	1:HHH:138:LEU:HB3	1.89	0.55
2:LLL:48:ILE:HA	2:LLL:53:VAL:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HHH:66:ARG:NH1	1:HHH:86:ASP:OD1	2.42	0.53
2:MMM:113:ALA:HB2	6:MMM:305:TRS:H22	1.92	0.52
1:III:71:ARG:HD3	1:III:73:ASN:OD1	2.10	0.51
2:LLL:13:ALA:HB3	2:LLL:78:LEU:HD22	1.93	0.51
2:LLL:85:ASP:OD2	2:LLL:103:LYS:HG2	2.11	0.51
1:III:66:ARG:NH1	1:III:86:ASP:OD1	2.43	0.51
1:HHH:71:ARG:HD3	1:HHH:73:ASN:OD1	2.10	0.50
2:LLL:184:GLU:O	2:LLL:188:SER:HB3	2.13	0.49
2:LLL:151:ALA:HB2	2:LLL:192:TYR:CE1	2.47	0.49
1:III:66:ARG:HD3	7:III:408:HOH:O	2.12	0.49
2:MMM:13:ALA:HB3	2:MMM:78:LEU:HD22	1.96	0.48
1:HHH:72:ASP:OD2	1:HHH:75:LYS:HD2	2.12	0.48
1:III:72:ASP:OD2	1:III:75:LYS:HD2	2.13	0.48
1:III:6:GLU:OE2	1:III:90:TYR:O	2.32	0.48
2:MMM:184:GLU:O	2:MMM:188:SER:HB3	2.13	0.47
1:III:178:LEU:C	1:III:178:LEU:CD1	2.83	0.46
2:LLL:167:LYS:HE3	2:LLL:171:ASN:HA	1.98	0.46
2:LLL:150:LYS:HB3	2:LLL:153:SER:HA	1.98	0.46
2:MMM:205:LYS:HA	2:MMM:205:LYS:HD2	1.75	0.46
1:HHH:153:SER:HB2	1:HHH:197:ASN:HB2	1.98	0.46
2:MMM:209:PRO:O	2:MMM:210:THR:C	2.54	0.45
2:MMM:151:ALA:HB2	2:MMM:192:TYR:CE1	2.52	0.45
2:LLL:2:GLN:HG2	2:LLL:97:VAL:HG12	1.99	0.45
1:HHH:17:SER:HA	1:HHH:82:MET:O	2.17	0.44
1:HHH:66:ARG:HD3	7:HHH:409:HOH:O	2.17	0.43
1:III:137:ALA:HB3	5:III:306:PEG:H41	1.99	0.43
1:III:17:SER:HA	1:III:82:MET:O	2.18	0.43
1:III:126:PRO:HD3	1:III:138:LEU:HB3	2.00	0.43
1:HHH:210:ARG:HH12	6:HHH:313:TRS:H11	1.84	0.43
2:MMM:87:TYR:CE2	2:MMM:101:GLY:HA3	2.54	0.43
1:HHH:6:GLU:OE2	1:HHH:107:THR:HG22	2.20	0.42
1:HHH:178:LEU:C	1:HHH:178:LEU:CD1	2.85	0.42
2:LLL:95(B):ASN:HD22	2:LLL:95(B):ASN:N	2.17	0.42
1:III:145:TYR:CE1	1:III:150:VAL:HG23	2.55	0.41
1:III:6:GLU:OE2	1:III:107:THR:HG22	2.19	0.41
1:HHH:145:TYR:CZ	1:HHH:150:VAL:CG1	3.03	0.41
2:LLL:157:LYS:H	2:LLL:157:LYS:HD2	1.85	0.41
2:MMM:197:THR:HA	2:MMM:201:SER:O	2.21	0.41
1:HHH:66:ARG:HH12	1:HHH:86:ASP:CG	2.24	0.41
2:MMM:12:SER:HB3	2:MMM:107:LEU:CD1	2.51	0.41
1:HHH:166:PHE:CZ	2:LLL:136:LEU:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:MMM:111:LYS:HD3	2:MMM:199:GLU:HG2	2.03	0.40
1:III:171:GLN:HG2	2:MMM:161:GLU:HG3	2.03	0.40
2:MMM:41:GLY:HA2	4:MMM:304:EDO:H21	2.03	0.40
1:III:201:LYS:N	1:III:202:PRO:CD	2.85	0.40
2:MMM:95(B):ASN:N	2:MMM:95(B):ASN:HD22	2.18	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	HHH	222/233 (95%)	210 (95%)	11 (5%)	1 (0%)	29	41
1	III	221/233 (95%)	212 (96%)	8 (4%)	1 (0%)	29	41
2	LLL	212/220 (96%)	199 (94%)	12 (6%)	1 (0%)	29	41
2	MMM	211/220 (96%)	196 (93%)	14 (7%)	1 (0%)	29	41
All	All	866/906 (96%)	817 (94%)	45 (5%)	4 (0%)	29	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	HHH	132	SER
2	MMM	84	ALA
2	LLL	84	ALA
1	III	55	GLY

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	HHH	186/191 (97%)	168 (90%)	18 (10%)	8 12
1	III	185/191 (97%)	163 (88%)	22 (12%)	5 6
2	LLL	180/185 (97%)	167 (93%)	13 (7%)	14 23
2	MMM	179/185 (97%)	168 (94%)	11 (6%)	18 30
All	All	730/752 (97%)	666 (91%)	64 (9%)	10 15

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	HHH	7	SER
1	HHH	28	THR
1	HHH	30	ARG
1	HHH	48	VAL
1	HHH	56	SER
1	HHH	129	LYS
1	HHH	130	SER
1	HHH	138	LEU
1	HHH	147	PRO
1	HHH	150	VAL
1	HHH	164	HIS
1	HHH	172	SER
1	HHH	178	LEU
1	HHH	199	ASN
1	HHH	209	LYS
1	HHH	210	ARG
1	HHH	215	SER
1	HHH	217	ASP
1	III	7	SER
1	III	25	SER
1	III	28	THR
1	III	48	VAL
1	III	56	SER
1	III	96	ARG
1	III	98	ASP
1	III	127	SER
1	III	128	SER
1	III	129	LYS
1	III	138	LEU
1	III	147	PRO

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Mol	Chain	Res	Type
1	III	149	PRO
1	III	161	SER
1	III	172	SER
1	III	178	LEU
1	III	186	SER
1	III	193	THR
1	III	199	ASN
1	III	209	LYS
1	III	212	GLU
1	III	215	SER
2	LLL	2	GLN
2	LLL	4	VAL
2	LLL	27	SER
2	LLL	56	SER
2	LLL	95(B)	ASN
2	LLL	103	LYS
2	LLL	104	LEU
2	LLL	123	SER
2	LLL	146	THR
2	LLL	157	LYS
2	LLL	176	SER
2	LLL	190	ARG
2	LLL	205	LYS
2	MMM	2	GLN
2	MMM	56	SER
2	MMM	94	LEU
2	MMM	103	LYS
2	MMM	123	SER
2	MMM	146	THR
2	MMM	157	LYS
2	MMM	167	LYS
2	MMM	199	GLU
2	MMM	203	VAL
2	MMM	205	LYS

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 3 are monoatomic - leaving 23 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	EDO	HHH	302	-	3,3,3	0.15	0	2,2,2	0.11	0
6	TRS	LLL	301	-	7,7,7	0.18	0	9,9,9	0.30	0
4	EDO	MMM	301	-	3,3,3	0.09	0	2,2,2	0.17	0
4	EDO	III	303	-	3,3,3	0.12	0	2,2,2	0.11	0
5	PEG	III	306	-	6,6,6	0.22	0	5,5,5	0.17	0
4	EDO	HHH	304	-	3,3,3	0.11	0	2,2,2	0.07	0
4	EDO	HHH	307	-	3,3,3	0.13	0	2,2,2	0.11	0
5	PEG	III	304	-	6,6,6	0.19	0	5,5,5	0.17	0
6	TRS	MMM	305	-	7,7,7	0.17	0	9,9,9	0.39	0
5	PEG	HHH	311	-	6,6,6	0.18	0	5,5,5	0.07	0
4	EDO	HHH	309	-	3,3,3	0.12	0	2,2,2	0.11	0
4	EDO	HHH	305	-	3,3,3	0.16	0	2,2,2	0.31	0
4	EDO	MMM	303	-	3,3,3	0.07	0	2,2,2	0.13	0
5	PEG	III	305	-	6,6,6	0.17	0	5,5,5	0.14	0
4	EDO	MMM	302	-	3,3,3	0.14	0	2,2,2	0.27	0
6	TRS	HHH	313	-	7,7,7	0.15	0	9,9,9	0.31	0
4	EDO	HHH	308	-	3,3,3	0.15	0	2,2,2	0.29	0
6	TRS	HHH	314	-	7,7,7	0.18	0	9,9,9	0.32	0
5	PEG	HHH	312	-	6,6,6	0.17	0	5,5,5	0.10	0
4	EDO	HHH	306	-	3,3,3	0.09	0	2,2,2	0.21	0
4	EDO	MMM	304	-	3,3,3	0.08	0	2,2,2	0.19	0
4	EDO	HHH	310	-	3,3,3	0.08	0	2,2,2	0.14	0
4	EDO	HHH	303	-	3,3,3	0.10	0	2,2,2	0.27	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	EDO	HHH	302	-	-	0/1/1/1	-
6	TRS	LLL	301	-	-	5/9/9/9	-
4	EDO	MMM	301	-	-	1/1/1/1	-
4	EDO	III	303	-	-	1/1/1/1	-
5	PEG	III	306	-	-	1/4/4/4	-
4	EDO	HHH	304	-	-	1/1/1/1	-
4	EDO	HHH	307	-	-	1/1/1/1	-
5	PEG	III	304	-	-	3/4/4/4	-
6	TRS	MMM	305	-	-	1/9/9/9	-
5	PEG	HHH	311	-	-	3/4/4/4	-
4	EDO	HHH	309	-	-	1/1/1/1	-
4	EDO	HHH	305	-	-	1/1/1/1	-
4	EDO	MMM	303	-	-	1/1/1/1	-
5	PEG	III	305	-	-	3/4/4/4	-
4	EDO	MMM	302	-	-	1/1/1/1	-
6	TRS	HHH	313	-	-	3/9/9/9	-
4	EDO	HHH	308	-	-	1/1/1/1	-
6	TRS	HHH	314	-	-	3/9/9/9	-
5	PEG	HHH	312	-	-	2/4/4/4	-
4	EDO	HHH	306	-	-	1/1/1/1	-
4	EDO	MMM	304	-	-	1/1/1/1	-
4	EDO	HHH	310	-	-	1/1/1/1	-
4	EDO	HHH	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	HHH	313	TRS	C1-C-C2-O2
6	HHH	314	TRS	C1-C-C2-O2
6	HHH	314	TRS	N-C-C2-O2
5	III	305	PEG	O2-C3-C4-O4
4	HHH	303	EDO	O1-C1-C2-O2
4	HHH	304	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	HHH	308	EDO	O1-C1-C2-O2
4	HHH	310	EDO	O1-C1-C2-O2
4	MMM	302	EDO	O1-C1-C2-O2
4	MMM	303	EDO	O1-C1-C2-O2
6	HHH	313	TRS	C3-C-C2-O2
5	HHH	312	PEG	O1-C1-C2-O2
5	III	305	PEG	O1-C1-C2-O2
5	III	306	PEG	O2-C3-C4-O4
4	HHH	306	EDO	O1-C1-C2-O2
5	HHH	311	PEG	O2-C3-C4-O4
4	MMM	304	EDO	O1-C1-C2-O2
5	HHH	311	PEG	C4-C3-O2-C2
5	HHH	312	PEG	O2-C3-C4-O4
6	HHH	314	TRS	C3-C-C2-O2
6	LLL	301	TRS	C1-C-C3-O3
6	LLL	301	TRS	N-C-C3-O3
5	III	304	PEG	C4-C3-O2-C2
5	III	304	PEG	O1-C1-C2-O2
5	III	304	PEG	O2-C3-C4-O4
4	HHH	309	EDO	O1-C1-C2-O2
4	III	303	EDO	O1-C1-C2-O2
6	LLL	301	TRS	C2-C-C3-O3
5	HHH	311	PEG	O1-C1-C2-O2
5	III	305	PEG	C4-C3-O2-C2
4	HHH	307	EDO	O1-C1-C2-O2
4	MMM	301	EDO	O1-C1-C2-O2
6	HHH	313	TRS	N-C-C2-O2
6	LLL	301	TRS	C3-C-C2-O2
6	LLL	301	TRS	N-C-C2-O2
6	MMM	305	TRS	C2-C-C3-O3
4	HHH	305	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	III	306	PEG	1	0
6	MMM	305	TRS	1	0
6	HHH	313	TRS	1	0
4	MMM	304	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	HHH	224/233 (96%)	0.12	2 (0%)	84	82	46, 58, 89, 147	0
1	III	223/233 (95%)	0.05	4 (1%)	68	66	46, 59, 99, 129	0
2	LLL	214/220 (97%)	0.19	11 (5%)	28	26	52, 73, 106, 136	0
2	MMM	213/220 (96%)	0.10	10 (4%)	31	30	52, 71, 91, 126	0
All	All	874/906 (96%)	0.11	27 (3%)	49	47	46, 64, 99, 147	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	LLL	2	GLN	10.5
2	MMM	2	GLN	6.4
1	HHH	217	ASP	4.4
2	MMM	192	TYR	3.8
1	III	216	CYS	3.7
2	MMM	190	ARG	3.5
1	III	214	LYS	3.4
2	LLL	3	SER	3.4
2	MMM	210	THR	3.3
2	LLL	186	TRP	3.0
1	HHH	129	LYS	3.0
2	LLL	190	ARG	2.9
2	LLL	192	TYR	2.9
2	LLL	157	LYS	2.9
2	MMM	157	LYS	2.8
2	LLL	211	GLU	2.8
2	LLL	148	ALA	2.8
2	MMM	156	VAL	2.8
2	MMM	153	SER	2.7
2	LLL	147	VAL	2.7
2	MMM	148	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	LLL	4	VAL	2.4
2	MMM	94	LEU	2.2
1	III	129	LYS	2.2
2	MMM	184	GLU	2.1
2	LLL	153	SER	2.1
1	III	27	PHE	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 monosaccharides 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(Å^2)	Q<0.9
4	EDO	MMM	302	4/4	0.43	0.43	55,96,97,97	1
4	EDO	MMM	304	4/4	0.65	0.22	55,84,86,87	1
4	EDO	HHH	306	4/4	0.66	0.22	55,82,88,88	1
5	PEG	III	304	7/7	0.66	0.30	55,81,93,94	1
5	PEG	III	305	7/7	0.67	0.31	55,92,96,96	1
6	TRS	HHH	314	8/8	0.67	0.40	55,102,118,120	2
5	PEG	HHH	312	7/7	0.68	0.34	55,94,96,101	1
4	EDO	HHH	308	4/4	0.70	0.32	55,79,83,84	1
5	PEG	HHH	311	7/7	0.70	0.22	55,96,113,115	17
6	TRS	MMM	305	8/8	0.74	0.30	55,95,117,120	2
6	TRS	HHH	313	8/8	0.79	0.24	55,89,98,103	2
6	TRS	LLL	301	8/8	0.80	0.22	55,85,96,97	2
4	EDO	MMM	303	4/4	0.81	0.17	55,77,91,94	1
4	EDO	HHH	309	4/4	0.84	0.16	55,74,76,79	1
4	EDO	HHH	304	4/4	0.85	0.20	55,81,82,83	1
5	PEG	III	306	7/7	0.86	0.24	55,95,101,103	1
4	EDO	III	303	4/4	0.88	0.14	55,68,71,72	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	HHH	310	4/4	0.89	0.15	55,83,84,85	1
3	CL	III	302	1/1	0.89	0.14	79,79,79,79	0
4	EDO	HHH	302	4/4	0.91	0.25	55,72,76,79	1
4	EDO	HHH	303	4/4	0.91	0.15	55,64,65,67	1
4	EDO	HHH	305	4/4	0.92	0.16	55,78,80,81	1
3	CL	III	301	1/1	0.92	0.19	56,56,56,56	1
4	EDO	HHH	307	4/4	0.93	0.14	55,77,78,79	1
4	EDO	MMM	301	4/4	0.97	0.16	55,65,70,71	1
3	CL	HHH	301	1/1	0.99	0.34	55,55,55,55	1

6.5 Other polymers (i)

There are no such residues in this entry.