Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:40 PM BST

PDB ID	:	6O2A
Title	:	Crystal structure of 4493 Fab in complex with circumsporozoite protein NDN and anti-kappa VHH domain
Authors	:	Scally, S.W.; Bosch, A.; Prieto, K.; Murugan, R.; Wardemann, H.; Julien, J.P.
Deposited on	:	2019-02-22
Resolution	:	2.15 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 ①) were used in the production of this report:

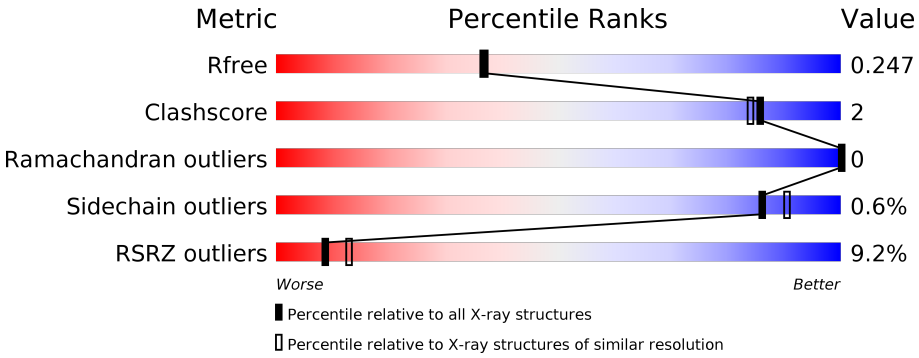
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	225	7% 93% 7%
1	C	225	13% 93% 5%
1	H	225	5% 93% 5%
1	O	225	4% 94%
2	B	215	6% 95% 5%
2	D	215	7% 93% 6%

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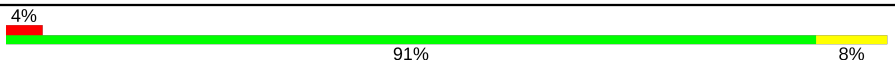
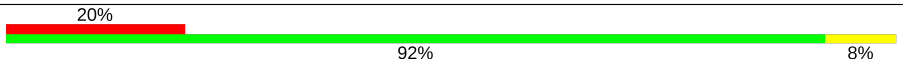
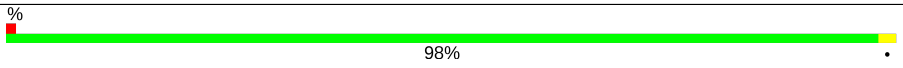
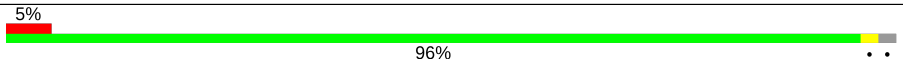
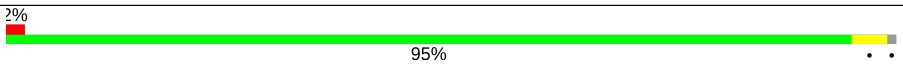
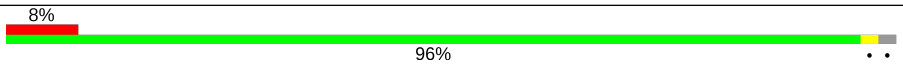
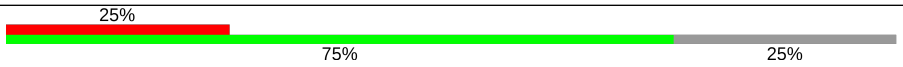
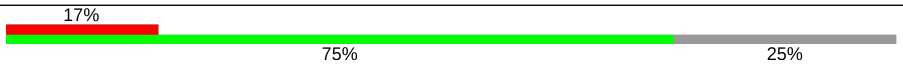
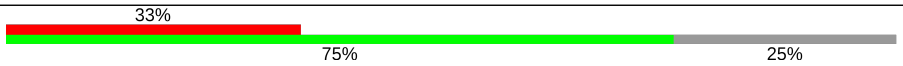
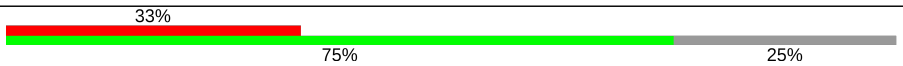
Mol	Chain	Length	Quality of chain
2	I	215	
2	P	215	
3	E	121	
3	J	121	
3	M	121	
3	N	121	
4	F	12	
4	G	12	
4	K	12	
4	L	12	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17037 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 4493 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1667	1048	284	328	7			
1	C	221	Total	C	N	O	S	0	1	0
			1646	1036	282	322	6			
1	H	221	Total	C	N	O	S	0	1	0
			1650	1039	283	322	6			
1	O	220	Total	C	N	O	S	0	1	0
			1645	1036	282	321	6			

- Molecule 2 is a protein called 4493 Kappa light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1650	1032	279	334	5			
2	D	214	Total	C	N	O	S	0	0	0
			1644	1029	278	333	4			
2	I	214	Total	C	N	O	S	0	0	0
			1638	1026	275	333	4			
2	P	214	Total	C	N	O	S	0	0	0
			1632	1023	272	333	4			

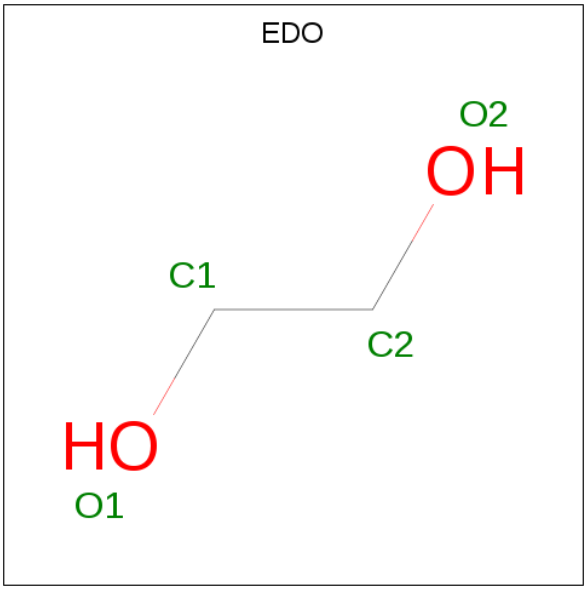
- Molecule 3 is a protein called Anti-kappa VHH domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			719	436	136	145	2			
3	M	120	Total	C	N	O	S	0	0	0
			713	433	135	143	2			
3	N	119	Total	C	N	O	S	0	0	0
			708	430	134	142	2			
3	J	119	Total	C	N	O	S	0	0	0
			708	430	134	142	2			

- Molecule 4 is a protein called Circumsporozoite protein.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	F	9	Total C N O 66 38 13 15	0	0	0
4	G	9	Total C N O 66 38 13 15	0	0	0
4	K	9	Total C N O 66 38 13 15	0	0	0
4	L	9	Total C N O 66 38 13 15	0	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0
5	O	1	Total C O 4 2 2	0	0
5	P	1	Total C O 4 2 2	0	0
5	P	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	N	1	Total C O 4 2 2	0	0
5	N	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	85	Total O 85 85	0	0
6	B	94	Total O 94 94	0	0
6	C	64	Total O 64 64	0	0
6	D	67	Total O 67 67	0	0
6	H	96	Total O 96 96	0	0
6	I	73	Total O 73 73	0	0
6	O	86	Total O 86 86	0	0
6	P	45	Total O 45 45	0	0

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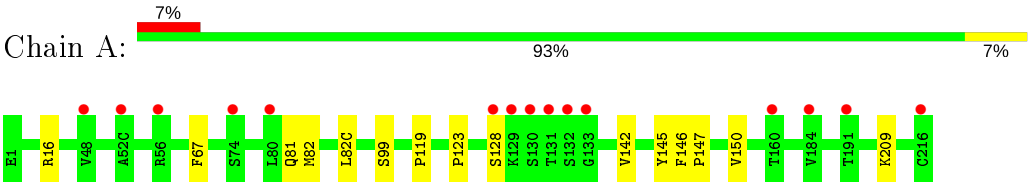
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	25	Total O 25 25	0	0
6	F	1	Total O 1 1	0	0
6	G	2	Total O 2 2	0	0
6	K	4	Total O 4 4	0	0
6	L	1	Total O 1 1	0	0
6	M	8	Total O 8 8	0	0
6	N	14	Total O 14 14	0	0
6	J	16	Total O 16 16	0	0

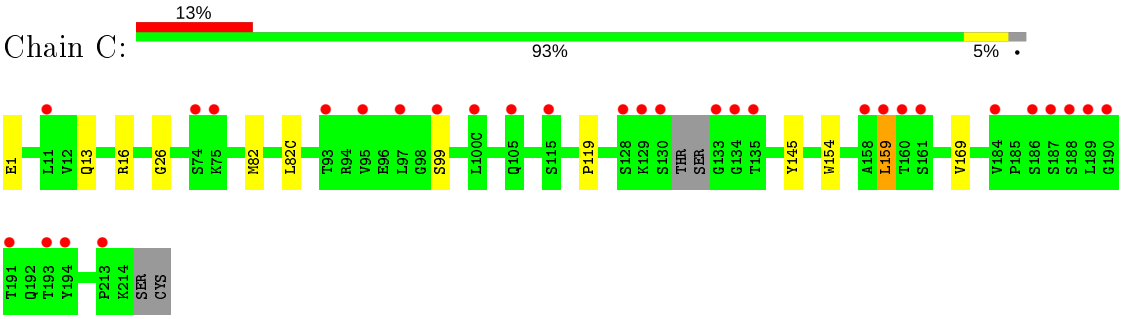
3 Residue-property plots (i)

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.

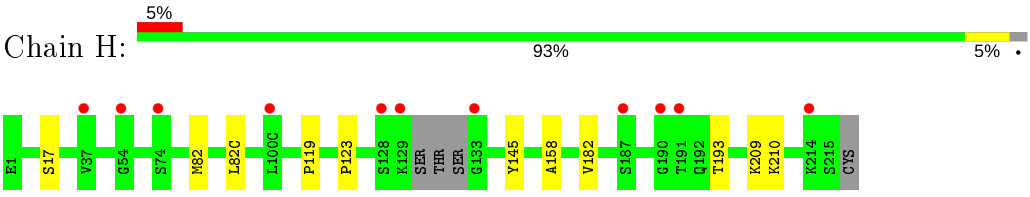
- Molecule 1: 4493 Fab heavy chain



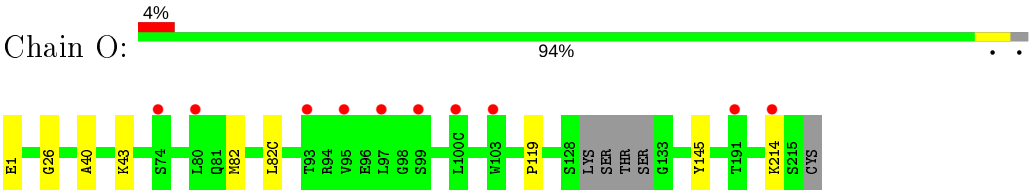
- Molecule 1: 4493 Fab heavy chain



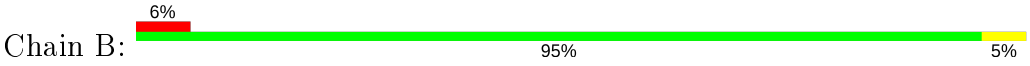
- Molecule 1: 4493 Fab heavy chain

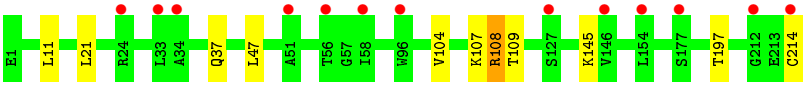


- Molecule 1: 4493 Fab heavy chain



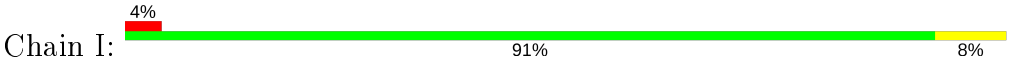
- Molecule 2: 4493 Kappa light chain

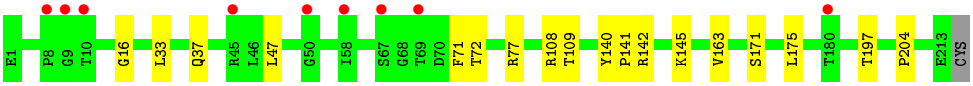




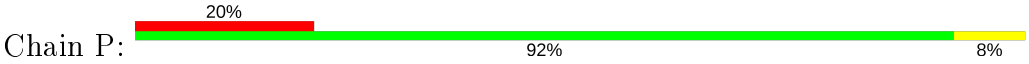
• Molecule 2: 4493 Kappa light chain

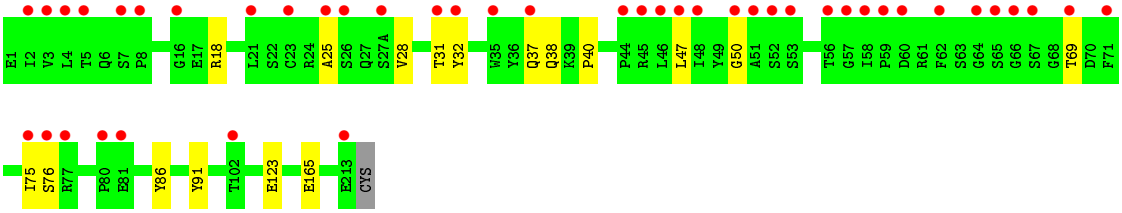
• Molecule 2: 4493 Kappa light chain



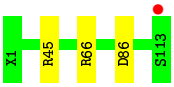


• Molecule 2: 4493 Kappa light chain

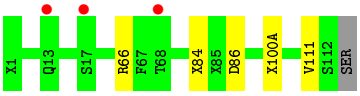




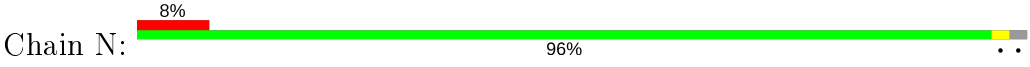
• Molecule 3: Anti-kappa VHH domain

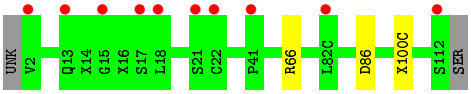


• Molecule 3: Anti-kappa VHH domain



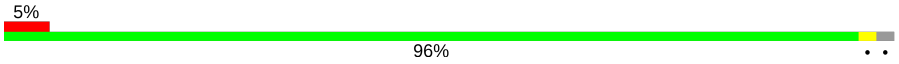
• Molecule 3: Anti-kappa VHH domain

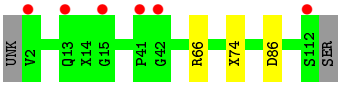




• Molecule 3: Anti-kappa VHH domain

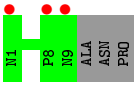
Chain J:





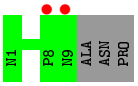
• Molecule 4: Circumsporozoite protein

Chain F:



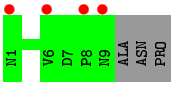
• Molecule 4: Circumsporozoite protein

Chain G:



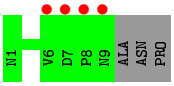
• Molecule 4: Circumsporozoite protein

Chain K:



• Molecule 4: Circumsporozoite protein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	82.65Å 90.73Å 92.52Å 89.38° 64.29° 76.88°	Depositor
Resolution (Å)	29.41 – 2.15 29.41 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.41-2.15) 93.0 (29.41-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.193 , 0.221 0.222 , 0.247	Depositor DCC
R_{free} test set	1357 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17037	wwPDB-VP
Average B, all atoms (Å^2)	54.0	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 41.66 % 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 2.2842e-04. 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: 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	0.26	0/1705	0.47	0/2318
1	C	0.26	0/1686	0.51	1/2292 (0.0%)
1	H	0.27	0/1690	0.48	0/2296
1	O	0.28	0/1685	0.48	0/2289
2	B	0.26	0/1687	0.48	0/2292
2	D	0.26	0/1681	0.47	0/2284
2	I	0.26	0/1675	0.48	0/2277
2	P	0.27	0/1669	0.49	0/2270
3	E	0.26	0/348	0.52	0/433
3	J	0.25	0/342	0.51	0/425
3	M	0.26	0/342	0.50	0/425
3	N	0.25	0/342	0.50	0/425
4	F	0.26	0/67	0.43	0/93
4	G	0.27	0/67	0.44	0/93
4	K	0.26	0/67	0.45	0/93
4	L	0.26	0/67	0.44	0/93
All	All	0.26	0/15120	0.48	1/20398 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	159	LEU	CA-CB-CG	6.50	130.25	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1667	0	1645	8	0
1	C	1646	0	1620	11	0
1	H	1650	0	1631	6	0
1	O	1645	0	1629	4	0
2	B	1650	0	1598	6	0
2	D	1644	0	1594	9	0
2	I	1638	0	1583	10	0
2	P	1632	0	1572	13	0
3	E	719	0	413	2	0
3	J	708	0	405	2	0
3	M	713	0	409	3	0
3	N	708	0	405	2	0
4	F	66	0	58	0	0
4	G	66	0	58	0	0
4	K	66	0	58	0	0
4	L	66	0	58	0	0
5	A	4	0	6	1	0
5	B	16	0	24	0	0
5	C	12	0	18	1	0
5	D	12	0	18	2	0
5	F	4	0	6	1	0
5	H	4	0	6	1	0
5	N	8	0	12	2	0
5	O	4	0	6	0	0
5	P	8	0	12	0	0
6	A	85	0	0	0	0
6	B	94	0	0	1	0
6	C	64	0	0	0	0
6	D	67	0	0	0	0
6	E	25	0	0	1	0
6	F	1	0	0	0	0
6	G	2	0	0	0	0
6	H	96	0	0	0	0
6	I	73	0	0	0	0
6	J	16	0	0	0	0
6	K	4	0	0	0	0
6	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	8	0	0	0	0
6	N	14	0	0	0	0
6	O	86	0	0	0	0
6	P	45	0	0	0	0
All	All	17037	0	14844	69	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 2.

All (69) 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:P:40:PRO:HG3	2:P:165:GLU:HG2	1.66	0.78
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.74	0.69
1:C:159:LEU:HD12	2:P:18:ARG:HH22	1.60	0.67
2:I:145:LYS:HB3	2:I:197:THR:HG22	1.76	0.66
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.80	0.64
2:I:37:GLN:HB2	2:I:47:LEU:HD11	1.81	0.63
1:H:17:SER:HB2	5:H:301:EDO:H12	1.82	0.61
2:I:204:PRO:HG3	5:N:201:EDO:H12	1.83	0.61
1:C:154:TRP:HB3	1:C:159:LEU:HD23	1.83	0.59
1:C:169:VAL:HG22	5:D:301:EDO:H11	1.84	0.59
3:N:66:ARG:NH2	3:N:86:ASP:OD1	2.35	0.59
1:C:159:LEU:HA	2:P:18:ARG:NH2	2.16	0.59
2:P:37:GLN:HB2	2:P:47:LEU:HD11	1.84	0.58
2:I:108:ARG:NH1	2:I:109:THR:O	2.35	0.58
1:C:159:LEU:CD1	2:P:18:ARG:HH22	2.16	0.58
1:C:16:ARG:HH21	5:C:401:EDO:H12	1.68	0.57
1:H:193:THR:HG23	1:H:210:LYS:HE3	1.87	0.56
3:M:66:ARG:NH2	3:M:86:ASP:OD1	2.33	0.56
2:P:18:ARG:HG3	2:P:75:ILE:O	2.07	0.55
3:J:66:ARG:NH2	3:J:86:ASP:OD1	2.32	0.55
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.89	0.55
2:B:108:ARG:HD3	2:B:109:THR:O	2.07	0.55
2:I:108:ARG:HD2	2:I:171:SER:HB2	1.92	0.52
1:O:119:PRO:HB3	1:O:145:TYR:HB3	1.92	0.51
1:A:99:SER:HA	5:F:401:EDO:H11	1.92	0.51
3:E:66:ARG:NH2	3:E:86:ASP:OD1	2.38	0.51
1:H:82:MET:HE2	1:H:82(C):LEU:HD21	1.93	0.50
2:P:37:GLN:NE2	2:P:86:TYR:OH	2.44	0.50
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.96	0.48
2:D:76:SER:HB2	1:H:158:ALA:HB1	1.95	0.48
1:A:82:MET:HE2	1:A:82(C):LEU:HD21	1.97	0.47
1:H:123:PRO:HD3	1:H:209:LYS:HE2	1.96	0.47
1:A:16:ARG:HE	5:A:301:EDO:H12	1.80	0.47
2:D:197:THR:HG22	3:M:100(A):UNK:O	2.15	0.47
2:D:45:ARG:NH1	3:J:74:UNK:HA	2.30	0.46
2:B:11:LEU:HD11	2:B:104:VAL:HG22	1.98	0.46
1:O:40:ALA:HB3	1:O:43:LYS:HD3	1.97	0.46
2:P:37:GLN:HG2	2:P:38:GLN:N	2.31	0.46
2:I:33:LEU:HD22	2:I:71:PHE:CD2	2.51	0.46
1:C:159:LEU:HD13	2:P:18:ARG:HH12	1.81	0.46
2:P:31:THR:HA	2:P:50:GLY:HA2	1.97	0.45
2:I:163:VAL:HG22	2:I:175:LEU:HD12	1.99	0.45
2:I:16:GLY:HA2	2:I:77:ARG:HG3	1.97	0.45
1:A:142:VAL:HG11	1:A:150:VAL:HG11	1.98	0.45
1:C:82:MET:HB3	1:C:82(C):LEU:HD21	1.98	0.45
2:P:25:ALA:O	2:P:69:THR:HG23	2.17	0.44
1:C:13:GLN:HB2	1:C:16:ARG:HG3	2.00	0.44
3:E:45:ARG:NH1	6:E:203:HOH:O	2.50	0.43
2:D:18:ARG:NH1	2:D:20:THR:OG1	2.50	0.43
3:M:84:UNK:HA	3:M:111:VAL:HB	2.01	0.43
2:I:142:ARG:NH1	2:I:163:VAL:HG21	2.34	0.42
3:N:100(C):UNK:HA	5:N:201:EDO:H11	2.00	0.42
1:C:1:GLU:O	1:C:26:GLY:HA3	2.18	0.42
2:D:16:GLY:HA2	2:D:77:ARG:HG3	2.01	0.42
1:O:82:MET:HB3	1:O:82(C):LEU:HD21	2.01	0.42
2:B:11:LEU:HD21	2:B:21:LEU:HG	2.01	0.42
2:I:140:TYR:CG	2:I:141:PRO:HA	2.55	0.41
1:A:123:PRO:HD3	1:A:209:LYS:HE2	2.02	0.41
2:B:107:LYS:NZ	6:B:406:HOH:O	2.53	0.41
2:D:33:LEU:HD22	2:D:71:PHE:CD2	2.56	0.41
1:O:1:GLU:O	1:O:26:GLY:HA3	2.20	0.41
2:D:175:LEU:HD12	5:D:302:EDO:H22	2.02	0.41
1:A:146:PHE:HA	1:A:147:PRO:HA	1.89	0.41
2:P:18:ARG:CD	2:P:76:SER:HA	2.51	0.41
1:A:67:PHE:HA	1:A:81:GLN:O	2.22	0.40
2:B:145:LYS:HB3	2:B:197:THR:OG1	2.22	0.40
2:D:33:LEU:HD22	2:D:71:PHE:CG	2.56	0.40
2:P:32:TYR:HA	2:P:91:TYR:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	223/225 (99%)	219 (98%)	4 (2%)	0	100	100
1	C	218/225 (97%)	215 (99%)	3 (1%)	0	100	100
1	H	218/225 (97%)	216 (99%)	2 (1%)	0	100	100
1	O	217/225 (96%)	213 (98%)	4 (2%)	0	100	100
2	B	213/215 (99%)	209 (98%)	4 (2%)	0	100	100
2	D	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
2	I	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
2	P	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
3	E	48/121 (40%)	48 (100%)	0	0	100	100
3	J	46/121 (38%)	46 (100%)	0	0	100	100
3	M	47/121 (39%)	47 (100%)	0	0	100	100
3	N	46/121 (38%)	46 (100%)	0	0	100	100
4	F	7/12 (58%)	7 (100%)	0	0	100	100
4	G	7/12 (58%)	7 (100%)	0	0	100	100
4	K	7/12 (58%)	7 (100%)	0	0	100	100
4	L	7/12 (58%)	7 (100%)	0	0	100	100
All	All	1940/2292 (85%)	1908 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	187/188 (100%)	186 (100%)	1 (0%)	88	92
1	C	183/188 (97%)	182 (100%)	1 (0%)	88	92
1	H	184/188 (98%)	183 (100%)	1 (0%)	88	92
1	O	184/188 (98%)	183 (100%)	1 (0%)	88	92
2	B	186/186 (100%)	184 (99%)	2 (1%)	73	78
2	D	185/186 (100%)	184 (100%)	1 (0%)	88	92
2	I	184/186 (99%)	183 (100%)	1 (0%)	88	92
2	P	183/186 (98%)	181 (99%)	2 (1%)	73	78
3	E	39/39 (100%)	39 (100%)	0	100	100
3	J	38/39 (97%)	38 (100%)	0	100	100
3	M	38/39 (97%)	38 (100%)	0	100	100
3	N	38/39 (97%)	38 (100%)	0	100	100
4	F	8/10 (80%)	8 (100%)	0	100	100
4	G	8/10 (80%)	8 (100%)	0	100	100
4	K	8/10 (80%)	8 (100%)	0	100	100
4	L	8/10 (80%)	8 (100%)	0	100	100
All	All	1661/1692 (98%)	1651 (99%)	10 (1%)	86	90

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	SER
2	B	108	ARG
2	B	214	CYS
1	C	99	SER
2	D	169	LYS
1	H	182	VAL
2	I	72	THR
1	O	214	LYS
2	P	28	VAL
2	P	123	GLU

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 monosaccharides in this entry.

5.6 Ligand geometry

18 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	$\#\|Z\| > 2$
5	EDO	N	201	-	3,3,3	0.49	0	2,2,2	0.15	0
5	EDO	C	401	-	3,3,3	0.43	0	2,2,2	0.45	0
5	EDO	B	302	-	3,3,3	0.43	0	2,2,2	0.33	0
5	EDO	O	301	-	3,3,3	0.46	0	2,2,2	0.35	0
5	EDO	P	401	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	B	303	-	3,3,3	0.46	0	2,2,2	0.35	0
5	EDO	D	303	-	3,3,3	0.46	0	2,2,2	0.32	0
5	EDO	N	202	-	3,3,3	0.46	0	2,2,2	0.30	0
5	EDO	A	301	-	3,3,3	0.43	0	2,2,2	0.41	0
5	EDO	C	402	-	3,3,3	0.46	0	2,2,2	0.35	0
5	EDO	H	301	-	3,3,3	0.44	0	2,2,2	0.31	0
5	EDO	D	301	-	3,3,3	0.44	0	2,2,2	0.38	0
5	EDO	B	304	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	C	403	-	3,3,3	0.46	0	2,2,2	0.32	0
5	EDO	P	402	-	3,3,3	0.45	0	2,2,2	0.30	0
5	EDO	F	401	-	3,3,3	0.44	0	2,2,2	0.37	0
5	EDO	B	301	-	3,3,3	0.44	0	2,2,2	0.37	0
5	EDO	D	302	-	3,3,3	0.46	0	2,2,2	0.26	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
5	EDO	N	201	-	-	0/1/1/1	-
5	EDO	C	401	-	-	0/1/1/1	-
5	EDO	B	302	-	-	0/1/1/1	-
5	EDO	O	301	-	-	0/1/1/1	-
5	EDO	P	401	-	-	0/1/1/1	-
5	EDO	B	303	-	-	0/1/1/1	-
5	EDO	D	303	-	-	0/1/1/1	-
5	EDO	N	202	-	-	0/1/1/1	-
5	EDO	A	301	-	-	0/1/1/1	-
5	EDO	C	402	-	-	1/1/1/1	-
5	EDO	H	301	-	-	1/1/1/1	-
5	EDO	D	301	-	-	0/1/1/1	-
5	EDO	B	304	-	-	0/1/1/1	-
5	EDO	C	403	-	-	1/1/1/1	-
5	EDO	P	402	-	-	0/1/1/1	-
5	EDO	F	401	-	-	0/1/1/1	-
5	EDO	B	301	-	-	0/1/1/1	-
5	EDO	D	302	-	-	0/1/1/1	-

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
5	H	301	EDO	O1-C1-C2-O2
5	C	403	EDO	O1-C1-C2-O2
5	C	402	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	201	EDO	2	0
5	C	401	EDO	1	0
5	A	301	EDO	1	0
5	H	301	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	301	EDO	1	0
5	F	401	EDO	1	0
5	D	302	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

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	225/225 (100%)	0.48	15 (6%) 17 24	34, 47, 76, 117	0
1	C	221/225 (98%)	0.76	30 (13%) 3 3	36, 52, 101, 140	0
1	H	221/225 (98%)	0.51	11 (4%) 28 37	33, 44, 66, 104	0
1	O	220/225 (97%)	0.54	10 (4%) 33 42	30, 48, 73, 106	0
2	B	215/215 (100%)	0.48	13 (6%) 21 29	30, 45, 68, 108	0
2	D	214/215 (99%)	0.49	16 (7%) 14 19	39, 52, 80, 104	0
2	I	214/215 (99%)	0.44	9 (4%) 36 45	33, 51, 70, 97	0
2	P	214/215 (99%)	1.05	44 (20%) 1 1	34, 56, 106, 124	0
3	E	49/121 (40%)	0.50	1 (2%) 65 72	34, 54, 84, 102	0
3	J	48/121 (39%)	0.63	6 (12%) 3 5	38, 55, 84, 108	0
3	M	48/121 (39%)	0.60	3 (6%) 20 27	45, 68, 88, 99	0
3	N	48/121 (39%)	1.09	10 (20%) 1 1	45, 65, 95, 105	0
4	F	9/12 (75%)	1.46	3 (33%) 0 0	48, 54, 79, 96	0
4	G	9/12 (75%)	1.43	2 (22%) 0 0	59, 63, 81, 109	0
4	K	9/12 (75%)	1.96	4 (44%) 0 0	43, 52, 76, 85	0
4	L	9/12 (75%)	2.08	4 (44%) 0 0	68, 77, 95, 96	0
All	All	1973/2292 (86%)	0.63	181 (9%) 9 13	30, 50, 87, 140	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	133	GLY	9.0
1	C	128	SER	8.2
1	A	216	CYS	8.1
2	P	25	ALA	7.6
1	C	187	SER	7.2

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Mol	Chain	Res	Type	RSRZ
1	C	190	GLY	6.8
3	N	112	SER	6.8
2	P	31	THR	6.7
1	C	133	GLY	6.7
2	P	2	ILE	6.4
1	C	189	LEU	6.3
4	K	9	ASN	6.2
2	P	51	ALA	6.1
1	A	132	SER	6.1
2	P	52	SER	6.1
3	J	112	SER	5.9
1	C	129	LYS	5.8
2	P	60	ASP	5.7
2	P	59	PRO	5.7
4	G	9	ASN	5.6
3	J	41	PRO	5.5
2	B	214	CYS	5.3
3	E	113	SER	5.2
2	P	67	SER	4.9
4	F	9	ASN	4.9
1	A	133	GLY	4.8
4	F	8	PRO	4.8
2	P	4	LEU	4.7
2	P	3	VAL	4.6
2	P	37	GLN	4.6
1	A	131	THR	4.5
1	C	74	SER	4.5
2	P	56	THR	4.4
2	P	80	PRO	4.3
2	P	57	GLY	4.3
1	H	128	SER	4.3
4	L	8	PRO	4.3
1	C	134	GLY	4.2
2	P	58	ILE	4.2
2	P	16	GLY	4.2
3	N	13	GLN	4.1
2	B	127	SER	4.0
1	O	99	SER	3.9
1	C	186	SER	3.9
1	C	160	THR	3.9
3	N	82(C)	LEU	3.9
2	P	53	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	O	95	VAL	3.7
3	N	41	PRO	3.7
2	D	51	ALA	3.6
4	K	8	PRO	3.6
2	P	7	SER	3.5
2	D	57	GLY	3.4
2	P	76	SER	3.4
2	D	25	ALA	3.4
3	N	15	GLY	3.3
1	C	159	LEU	3.3
2	P	5	THR	3.2
2	D	126	LYS	3.2
1	C	11	LEU	3.2
3	N	2	VAL	3.2
1	H	191	THR	3.2
4	L	9	ASN	3.2
1	O	100(C)	LEU	3.1
2	B	212	GLY	3.1
3	J	42	GLY	3.1
4	L	7	ASP	3.1
2	P	102	THR	3.0
3	M	13	GLN	3.0
1	A	130	SER	3.0
3	M	17	SER	3.0
2	D	46	LEU	3.0
2	P	46	LEU	3.0
2	I	9	GLY	2.9
2	I	8	PRO	2.9
3	J	13	GLN	2.9
1	A	74	SER	2.9
2	P	8	PRO	2.9
1	C	115	SER	2.9
2	D	58	ILE	2.9
2	D	52	SER	2.8
1	C	194	TYR	2.8
2	P	45	ARG	2.8
1	C	97	LEU	2.8
2	B	33	LEU	2.8
1	H	129	LYS	2.7
2	P	21	LEU	2.7
1	C	191	THR	2.7
1	H	214	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	I	45	ARG	2.7
2	P	44	PRO	2.7
3	J	2	VAL	2.7
2	P	75	ILE	2.7
2	D	125	LEU	2.7
4	K	1	ASN	2.7
1	C	100(C)	LEU	2.7
2	D	33	LEU	2.7
1	C	130	SER	2.6
2	P	66	GLY	2.6
1	C	188	SER	2.6
1	H	74	SER	2.6
2	B	34	ALA	2.6
1	C	193	THR	2.6
2	I	69	THR	2.6
2	P	48	ILE	2.6
1	A	160	THR	2.5
2	P	213	GLU	2.5
2	D	80	PRO	2.5
2	I	67	SER	2.5
2	P	32	TYR	2.5
1	O	214	LYS	2.5
2	P	27(A)	SER	2.5
1	H	54	GLY	2.5
3	N	22	CYS	2.5
1	C	135	THR	2.5
1	O	97	LEU	2.4
1	C	95	VAL	2.4
1	C	99	SER	2.4
4	G	8	PRO	2.4
1	H	100(C)	LEU	2.4
2	P	35	TRP	2.4
2	B	51	ALA	2.4
1	A	80	LEU	2.4
4	L	6	VAL	2.4
2	I	10	THR	2.4
2	B	154	LEU	2.3
2	P	81	GLU	2.3
1	O	93	THR	2.3
4	F	1	ASN	2.3
2	P	77	ARG	2.3
2	D	179	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	P	62	PHE	2.3
3	N	18	LEU	2.3
2	D	148	TRP	2.3
2	P	50	GLY	2.3
3	J	15	GLY	2.3
1	A	129	LYS	2.3
3	M	68	THR	2.3
3	N	17	SER	2.3
1	H	187	SER	2.3
2	P	64	GLY	2.3
1	A	56	ARG	2.3
1	C	105	GLN	2.3
1	O	191	THR	2.3
3	N	21	SER	2.2
1	C	158	ALA	2.2
1	H	190	GLY	2.2
2	I	58	ILE	2.2
2	D	178	THR	2.2
1	A	48	VAL	2.2
4	K	6	VAL	2.2
1	O	103	TRP	2.2
1	C	93	THR	2.2
1	O	74	SER	2.2
1	A	191	THR	2.2
2	D	1	GLU	2.2
2	P	47	LEU	2.2
2	B	24	ARG	2.2
2	P	26	SER	2.2
2	B	58	ILE	2.1
1	C	184	VAL	2.1
2	P	23	CYS	2.1
1	C	75	LYS	2.1
2	P	65	SER	2.1
2	D	169	LYS	2.1
1	C	161	SER	2.1
2	B	146	VAL	2.1
2	B	177	SER	2.1
2	P	71	PHE	2.1
2	I	180	THR	2.1
2	I	50	GLY	2.1
1	A	128	SER	2.1
1	C	213	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	80	LEU	2.0
2	D	70	ASP	2.0
1	A	52(C)	ALA	2.0
1	A	184	VAL	2.0
1	H	37	VAL	2.0
2	B	56	THR	2.0
2	P	69	THR	2.0
2	B	96	TRP	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, 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
5	EDO	D	303	4/4	0.64	0.16	68,69,72,74	0
5	EDO	N	202	4/4	0.67	0.20	71,73,76,76	0
5	EDO	D	301	4/4	0.68	0.31	57,59,61,62	0
5	EDO	C	403	4/4	0.68	0.32	77,79,79,79	0
5	EDO	B	304	4/4	0.70	0.26	70,71,71,74	0
5	EDO	D	302	4/4	0.73	0.22	62,63,65,71	0
5	EDO	N	201	4/4	0.74	0.33	63,63,63,68	0
5	EDO	B	303	4/4	0.79	0.26	76,78,80,80	0
5	EDO	C	401	4/4	0.81	0.35	63,65,67,67	0
5	EDO	H	301	4/4	0.84	0.24	43,47,52,58	0
5	EDO	O	301	4/4	0.88	0.29	65,66,67,73	0
5	EDO	C	402	4/4	0.89	0.30	57,62,68,72	0
5	EDO	P	401	4/4	0.90	0.14	45,46,49,58	0
5	EDO	F	401	4/4	0.91	0.14	59,61,62,67	0
5	EDO	A	301	4/4	0.91	0.28	61,61,63,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	B	302	4/4	0.93	0.22	69,70,71,73	0
5	EDO	P	402	4/4	0.93	0.19	49,63,68,72	0
5	EDO	B	301	4/4	0.94	0.26	46,49,52,61	0

6.5 Other polymers (i)

There are no such residues in this entry.