



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2021 – 04:10 PM JST

PDB ID : 7E72
Title : Crystal structure of Tie2-agonistic antibody in complex with human Tie2 Fn2-3
Authors : Kim, H.M.; Jo, G.H.; Hong, H.J.; Han, A.
Deposited on : 2021-02-25
Resolution : 2.09 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 : 2.23.2
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) : 2.23.2

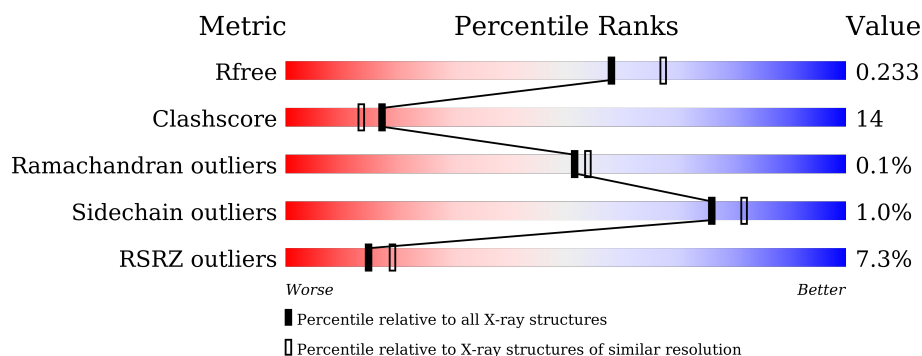
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	227	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 27%, orange 62%, yellow 84%, green 100%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 27% 62% 84% 12% . </div> </div>
1	C	227	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 16%, orange 69%, yellow 77%, green 100%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 16% 69% 77% 19% . </div> </div>
2	B	214	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 85%, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 85% 15% </div> </div>
2	D	214	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 86%, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 86% 14% </div> </div>
3	E	199	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 27%, orange 62%, yellow 84%, green 100%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 27% 62% 84% 12% .. </div> </div>
3	F	199	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 16%, orange 69%, yellow 77%, green 100%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 16% 69% 77% 19% .. </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	307	-	-	X	-
4	EDO	B	308	-	-	X	-
4	EDO	C	306	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10698 atoms, of which 204 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 the chimeric Fab fragment of 3H7 (heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1628	1024	273	322	9			
1	C	218	Total	C	N	O	S	0	0	0
			1628	1024	273	322	9			

- Molecule 2 is a protein called the chimeric Fab fragment of 3H7 (light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1643	1021	274	342	6			
2	D	214	Total	C	N	O	S	0	0	0
			1643	1021	274	342	6			

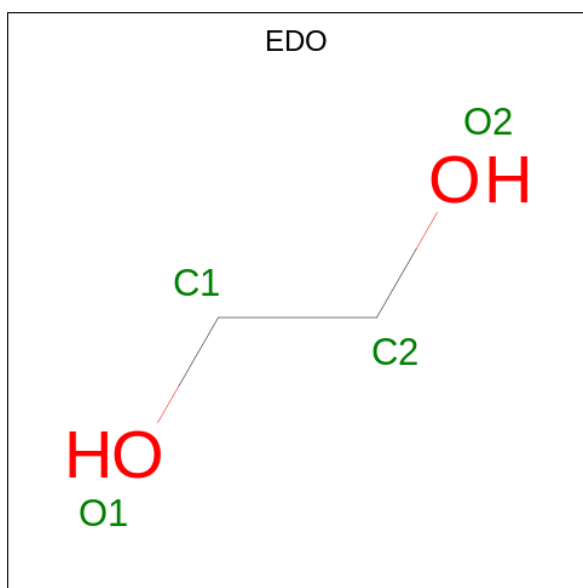
- Molecule 3 is a protein called Angiopoietin-1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	196	Total	C	N	O	S	0	0	0
			1540	972	264	303	1			
3	F	196	Total	C	N	O	S	0	0	0
			1539	975	264	299	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	537	GLY	-	expression tag	UNP Q02763
E	538	SER	-	expression tag	UNP Q02763
E	539	HIS	-	expression tag	UNP Q02763
E	540	MET	-	expression tag	UNP Q02763
F	537	GLY	-	expression tag	UNP Q02763
F	538	SER	-	expression tag	UNP Q02763
F	539	HIS	-	expression tag	UNP Q02763
F	540	MET	-	expression tag	UNP Q02763

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	E	1	Total	C	H	O	0	0
			10	2	6	2		
4	F	1	Total	C	H	O	0	0
			10	2	6	2		

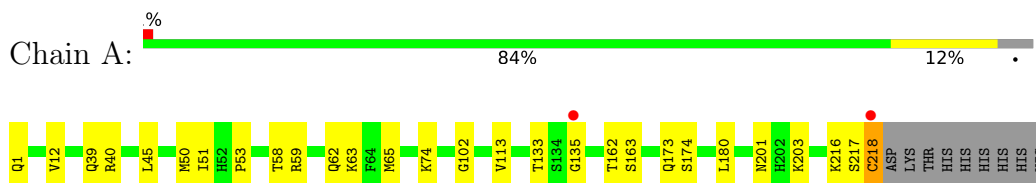
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	163	Total 163	O 163	0	0
5	B	177	Total 177	O 177	0	0
5	C	164	Total 164	O 164	0	0
5	D	174	Total 174	O 174	0	0
5	E	31	Total 31	O 31	0	0
5	F	28	Total 28	O 28	0	0

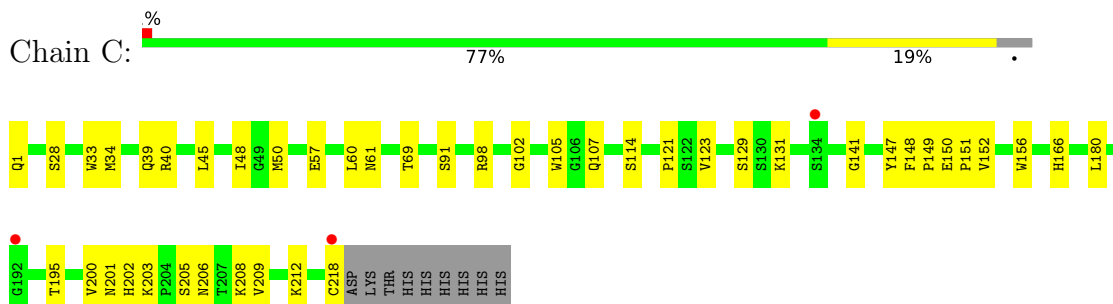
3 Residue-property plots

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.

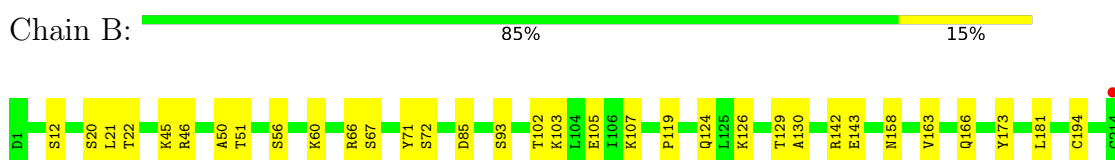
- Molecule 1: the chimeric Fab fragment of 3H7 (heavy chain)



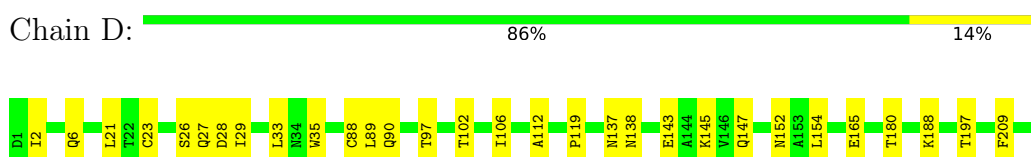
- Molecule 1: the chimeric Fab fragment of 3H7 (heavy chain)



- Molecule 2: the chimeric Fab fragment of 3H7 (light chain)

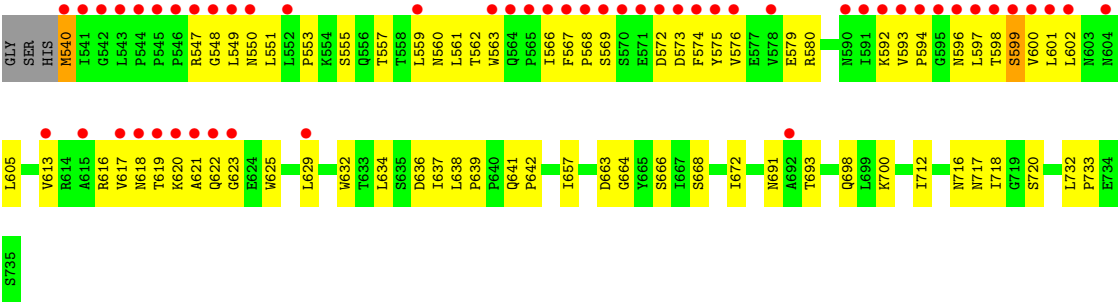


- Molecule 2: the chimeric Fab fragment of 3H7 (light chain)

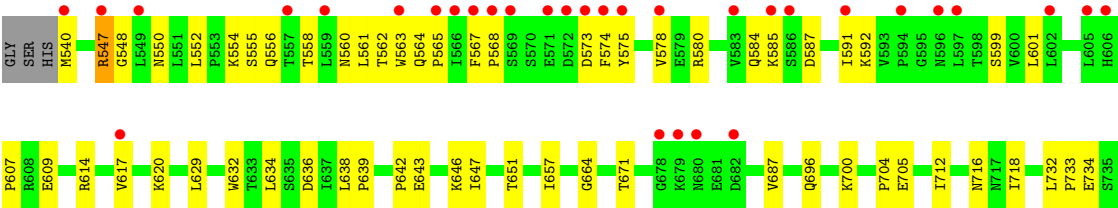


- Molecule 3: Angiopoietin-1 receptor





● Molecule 3: Angiopoietin-1 receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.08Å 77.34Å 121.85Å 103.82° 96.89° 90.59°	Depositor
Resolution (Å)	44.72 – 2.09 44.72 – 2.09	Depositor EDS
% Data completeness (in resolution range)	91.0 (44.72-2.09) 91.0 (44.72-2.09)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.183 , 0.233 0.183 , 0.233	Depositor DCC
R_{free} test set	2006 reflections (2.36%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10698	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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

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	0.41	0/1668	0.55	0/2272
1	C	0.42	0/1668	0.57	0/2272
2	B	0.46	1/1674 (0.1%)	0.60	0/2268
2	D	0.47	0/1674	0.61	0/2268
3	E	0.32	0/1575	0.54	0/2153
3	F	0.32	0/1574	0.50	0/2152
All	All	0.41	1/9833 (0.0%)	0.56	0/13385

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	194	CYS	CB-SG	-6.30	1.71	1.82

There are no bond angle outliers.

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	1628	0	1602	27	0
1	C	1628	0	1602	44	0
2	B	1643	0	1591	32	0
2	D	1643	0	1591	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1540	0	1507	88	0
3	F	1539	0	1519	56	0
4	A	40	60	60	8	0
4	B	44	66	66	18	0
4	C	24	36	36	11	0
4	D	20	30	30	6	0
4	E	4	6	6	0	0
4	F	4	6	6	1	0
5	A	163	0	0	3	0
5	B	177	0	0	2	0
5	C	164	0	0	4	0
5	D	174	0	0	3	0
5	E	31	0	0	2	0
5	F	28	0	0	2	0
All	All	10494	204	9616	269	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 14.

All (269) 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)
3:E:657:ILE:HD11	3:E:712:ILE:HD11	1.26	1.12
3:E:618:ASN:HB3	3:E:621:ALA:HB1	1.46	0.96
3:F:556:GLN:HB3	3:F:607:PRO:HB3	1.50	0.94
1:C:218:CYS:SG	2:D:214:CYS:HB3	2.07	0.94
2:D:143:GLU:OE1	5:D:401:HOH:O	1.85	0.94
3:E:562:THR:HG22	3:E:599:SER:HB2	1.53	0.91
1:C:218:CYS:SG	2:D:214:CYS:CB	2.60	0.90
1:C:69:THR:HG23	5:C:487:HOH:O	1.71	0.90
3:E:657:ILE:CD1	3:E:712:ILE:HD11	2.02	0.89
3:E:620:LYS:N	3:E:621:ALA:HA	1.89	0.88
3:E:572:ASP:HB2	3:E:573:ASP:O	1.75	0.87
3:E:549:LEU:HD22	3:E:561:LEU:HD11	1.56	0.84
3:F:564:GLN:HB3	3:F:565:PRO:HD2	1.60	0.83
2:B:60:LYS:O	5:B:401:HOH:O	1.98	0.82
2:B:12:SER:OG	2:B:105:GLU:OE2	1.97	0.81
3:E:547:ARG:CD	3:E:548:GLY:H	1.94	0.80
3:F:585:LYS:HE3	3:F:587:ASP:HB2	1.65	0.79
1:C:102:GLY:HA3	4:C:301:EDO:H11	1.64	0.79
3:E:563:TRP:O	3:E:598:THR:OG1	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:308:EDO:H22	2:B:119:PRO:HG2	1.67	0.77
2:D:90:GLN:HG3	2:D:97:THR:HG22	1.68	0.75
3:F:642:PRO:HG2	3:F:712:ILE:HG22	1.69	0.74
3:F:562:THR:HG22	3:F:599:SER:HB2	1.69	0.74
3:F:560:ASN:HD22	3:F:601:LEU:HD12	1.53	0.74
3:E:618:ASN:CB	3:E:621:ALA:HB1	2.18	0.73
3:E:540:MET:O	3:E:622:GLN:HB2	1.89	0.73
3:E:593:VAL:HG23	3:E:594:PRO:HD2	1.71	0.73
3:E:698:GLN:OE1	3:E:700:LYS:NZ	2.22	0.73
2:B:143:GLU:H	4:B:308:EDO:H22	1.54	0.72
1:A:53:PRO:O	1:A:74:LYS:NZ	2.23	0.71
3:E:551:LEU:HD22	3:E:613:VAL:CG2	2.21	0.71
3:E:557:THR:HG23	3:E:605:LEU:O	1.90	0.70
3:F:547:ARG:HB2	3:F:564:GLN:HB2	1.72	0.70
1:A:173:GLN:HB3	4:A:307:EDO:H12	1.74	0.70
3:F:614:ARG:NH1	5:F:901:HOH:O	2.17	0.70
1:A:135:GLY:HA2	5:A:401:HOH:O	1.91	0.70
2:B:105:GLU:HB3	4:B:311:EDO:H22	1.74	0.70
3:F:562:THR:HG22	3:F:599:SER:CB	2.22	0.69
1:C:107:GLN:O	4:C:302:EDO:O1	2.11	0.69
1:C:28:SER:OG	3:F:643:GLU:OE1	2.10	0.69
2:D:154:LEU:HD22	5:D:406:HOH:O	1.91	0.69
3:E:547:ARG:CD	3:E:548:GLY:N	2.56	0.68
3:E:576:VAL:HG23	3:E:616:ARG:O	1.93	0.68
2:B:143:GLU:HB3	4:B:308:EDO:H11	1.76	0.68
1:C:114:SER:HB2	4:C:306:EDO:H11	1.76	0.68
2:D:2:ILE:O	2:D:97:THR:HG21	1.94	0.68
2:B:142:ARG:NH2	2:B:163:VAL:HG11	2.09	0.67
1:C:123:VAL:HG21	1:C:209:VAL:HG11	1.77	0.66
1:C:129:SER:OG	1:C:131:LYS:HG2	1.94	0.66
3:F:584:GLN:HG3	3:F:609:GLU:HG3	1.77	0.66
2:D:90:GLN:CG	2:D:97:THR:HG22	2.25	0.65
3:E:572:ASP:HB3	3:E:620:LYS:HZ2	1.62	0.65
3:E:602:LEU:H	3:E:602:LEU:HD22	1.62	0.65
3:F:575:TYR:CE2	3:F:592:LYS:HE3	2.31	0.64
1:C:69:THR:HG22	5:C:547:HOH:O	1.97	0.64
3:E:562:THR:HG22	3:E:599:SER:CB	2.26	0.64
1:C:114:SER:HB2	4:C:306:EDO:C1	2.29	0.63
3:E:616:ARG:HG3	3:E:625:TRP:CE3	2.34	0.63
1:C:123:VAL:HG21	1:C:209:VAL:CG1	2.29	0.63
3:E:547:ARG:HD2	3:E:548:GLY:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:585:LYS:CE	3:F:587:ASP:HB2	2.29	0.62
3:E:639:PRO:HD3	3:E:716:ASN:OD1	1.99	0.62
1:A:162:THR:HG22	5:A:493:HOH:O	2.00	0.61
3:E:572:ASP:OD2	3:E:574:PHE:HA	2.01	0.61
3:F:548:GLY:O	3:F:563:TRP:HA	2.00	0.61
3:E:572:ASP:HB3	3:E:620:LYS:NZ	2.14	0.61
3:E:641:GLN:NE2	5:E:903:HOH:O	2.34	0.60
1:A:201:ASN:HD21	1:A:203:LYS:HG3	1.66	0.60
3:E:551:LEU:HD22	3:E:613:VAL:HG22	1.84	0.60
1:C:201:ASN:HD21	1:C:203:LYS:HG3	1.66	0.60
3:E:575:TYR:HD2	3:E:592:LYS:HZ3	1.48	0.60
1:C:48:ILE:O	1:C:60:LEU:HD12	2.02	0.60
3:E:572:ASP:HB2	3:E:573:ASP:C	2.21	0.60
3:E:636:ASP:OD1	3:E:637:ILE:HG12	2.01	0.60
3:F:578:VAL:HG23	3:F:591:ILE:HB	1.83	0.59
3:E:566:ILE:HD12	3:E:566:ILE:H	1.67	0.59
3:E:572:ASP:OD2	3:E:619:THR:HA	2.03	0.58
3:E:617:VAL:O	3:E:623:GLY:HA3	2.03	0.58
1:C:123:VAL:CG2	1:C:209:VAL:HG11	2.34	0.58
3:F:584:GLN:CG	3:F:609:GLU:HG3	2.33	0.58
3:F:651:THR:HA	3:F:732:LEU:HD12	1.86	0.58
1:C:201:ASN:ND2	1:C:203:LYS:HG3	2.19	0.57
1:C:39:GLN:HB2	1:C:45:LEU:HD23	1.85	0.57
3:E:550:ASN:O	3:E:561:LEU:HA	2.05	0.57
3:E:566:ILE:HD12	3:E:566:ILE:N	2.20	0.57
1:A:39:GLN:HB2	1:A:45:LEU:HD23	1.85	0.57
3:E:547:ARG:CG	3:E:548:GLY:H	2.17	0.57
3:F:554:LYS:O	3:F:555:SER:HB3	2.05	0.57
3:F:700:LYS:N	4:F:801:EDO:O2	2.37	0.56
1:A:1:GLN:OE1	1:A:1:GLN:N	2.29	0.56
2:D:165:GLU:CD	2:D:165:GLU:H	2.08	0.56
2:D:90:GLN:HE21	2:D:97:THR:HG22	1.71	0.56
3:F:564:GLN:HB3	3:F:565:PRO:CD	2.34	0.56
3:E:616:ARG:HG3	3:E:625:TRP:CD2	2.41	0.56
3:E:551:LEU:HD22	3:E:613:VAL:HG21	1.88	0.56
3:E:593:VAL:HG11	3:E:600:VAL:CG2	2.37	0.55
1:A:180:LEU:C	1:A:180:LEU:HD12	2.27	0.55
3:E:637:ILE:HG22	3:E:638:LEU:N	2.22	0.55
2:D:106:ILE:HD12	4:D:301:EDO:H21	1.89	0.55
3:E:594:PRO:HB2	3:E:596:ASN:OD1	2.07	0.55
3:F:705:GLU:HG2	3:F:733:PRO:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:GLN:HB2	2:D:23:CYS:SG	2.47	0.55
3:F:548:GLY:N	3:F:564:GLN:HG3	2.22	0.54
3:F:620:LYS:HE3	5:F:925:HOH:O	2.07	0.54
1:A:133:THR:N	4:A:309:EDO:O2	2.31	0.54
2:B:45:LYS:HG3	4:B:307:EDO:H22	1.88	0.54
3:F:638:LEU:HD13	3:F:718:ILE:HG22	1.89	0.54
1:A:102:GLY:HA3	4:A:303:EDO:C2	2.37	0.54
2:B:21:LEU:O	2:B:72:SER:HA	2.08	0.54
3:E:632:TRP:CD2	3:E:664:GLY:HA2	2.43	0.54
1:C:148:PHE:HE1	4:C:306:EDO:H12	1.72	0.54
3:E:593:VAL:CG2	3:E:594:PRO:HD2	2.38	0.53
2:B:142:ARG:HG2	4:B:305:EDO:H12	1.90	0.53
1:C:33:TRP:HB3	1:C:50:MET:HE2	1.90	0.53
3:E:691:ASN:CG	3:E:693:THR:HG22	2.28	0.53
3:F:578:VAL:CG2	3:F:591:ILE:HB	2.39	0.53
1:A:217:SER:O	1:A:218:CYS:HB2	2.07	0.53
2:B:20:SER:O	4:B:302:EDO:O2	2.23	0.53
3:E:547:ARG:HD3	3:E:548:GLY:H	1.74	0.53
2:B:124:GLN:HG2	2:B:129:THR:O	2.08	0.53
1:A:62:GLN:HA	1:A:65:MET:HG2	1.90	0.53
3:E:555:SER:HA	3:E:634:LEU:HD12	1.91	0.52
3:E:636:ASP:O	3:E:637:ILE:HD13	2.09	0.52
2:B:158:ASN:ND2	4:B:310:EDO:O1	2.34	0.52
3:E:575:TYR:CD2	3:E:592:LYS:HD2	2.45	0.52
1:A:40:ARG:HH21	1:A:40:ARG:HG3	1.74	0.52
1:C:203:LYS:HE2	1:C:208:LYS:NZ	2.24	0.52
1:C:147:TYR:CE1	1:C:152:VAL:HG13	2.45	0.52
3:F:580:ARG:HD2	3:F:580:ARG:O	2.10	0.52
3:E:691:ASN:ND2	3:E:693:THR:HG22	2.25	0.52
3:F:575:TYR:CZ	3:F:592:LYS:HE3	2.45	0.52
3:E:579:GLU:O	3:E:613:VAL:HA	2.10	0.51
1:C:166:HIS:ND1	4:C:304:EDO:H21	2.25	0.51
3:E:561:LEU:O	3:E:599:SER:HA	2.10	0.51
3:E:566:ILE:HG22	3:E:567:PHE:N	2.25	0.51
3:E:619:THR:OG1	3:E:620:LYS:N	2.43	0.51
3:E:617:VAL:O	3:E:617:VAL:HG23	2.11	0.51
3:E:691:ASN:OD1	3:E:693:THR:HG22	2.11	0.51
3:E:663:ASP:OD1	3:E:664:GLY:N	2.44	0.50
1:A:40:ARG:HG3	1:A:40:ARG:NH2	2.26	0.50
2:B:21:LEU:HD22	2:B:102:THR:HG21	1.93	0.50
2:D:180:THR:HG21	4:D:302:EDO:O1	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:557:THR:O	3:E:557:THR:HG22	2.11	0.50
3:E:553:PRO:HA	3:E:559:LEU:HG	1.94	0.50
3:E:642:PRO:HG2	3:E:712:ILE:HG22	1.92	0.50
3:F:558:THR:HG23	3:F:601:LEU:HG	1.93	0.50
1:A:51:ILE:HG13	1:A:58:THR:HG22	1.94	0.49
1:C:40:ARG:NH2	1:C:91:SER:O	2.45	0.49
3:F:585:LYS:HE3	3:F:587:ASP:CB	2.40	0.49
3:F:580:ARG:NH1	3:F:587:ASP:OD2	2.33	0.49
3:F:638:LEU:CD1	3:F:718:ILE:HG22	2.42	0.49
3:F:562:THR:HG22	3:F:599:SER:HB3	1.95	0.49
1:C:180:LEU:HD12	1:C:180:LEU:C	2.33	0.49
1:C:195:THR:OG1	1:C:212:LYS:HE3	2.13	0.49
2:D:145:LYS:HB3	2:D:197:THR:HB	1.95	0.49
3:E:563:TRP:HH2	3:E:600:VAL:HG23	1.77	0.49
2:B:143:GLU:CB	4:B:308:EDO:H11	2.42	0.49
2:D:27:GLN:O	2:D:29:ILE:N	2.46	0.49
3:E:618:ASN:OD1	3:E:623:GLY:N	2.40	0.49
3:F:568:PRO:HG3	3:F:574:PHE:CE1	2.47	0.49
1:C:166:HIS:CE1	4:C:304:EDO:H21	2.48	0.49
1:C:200:VAL:HB	1:C:209:VAL:HG13	1.95	0.48
3:E:596:ASN:OD1	3:E:596:ASN:N	2.46	0.48
3:F:632:TRP:CD2	3:F:664:GLY:HA2	2.47	0.48
3:F:638:LEU:HD13	3:F:718:ILE:CG2	2.43	0.48
1:A:12:VAL:O	1:A:113:VAL:HA	2.12	0.48
3:E:555:SER:CA	3:E:634:LEU:HD12	2.43	0.48
3:F:556:GLN:OE1	3:F:636:ASP:HA	2.12	0.48
1:C:121:PRO:HB3	1:C:147:TYR:HB3	1.96	0.48
2:D:147:GLN:HB3	5:D:406:HOH:O	2.13	0.48
1:C:1:GLN:NE2	5:C:405:HOH:O	2.47	0.47
3:E:613:VAL:HG23	3:E:629:LEU:HB2	1.97	0.47
1:C:200:VAL:O	1:C:208:LYS:HA	2.14	0.47
3:E:634:LEU:HA	3:E:666:SER:OG	2.15	0.47
3:E:600:VAL:HG12	3:E:601:LEU:N	2.29	0.47
3:E:540:MET:C	3:E:622:GLN:HB2	2.34	0.47
3:F:647:ILE:N	3:F:647:ILE:HD12	2.30	0.46
2:D:138:ASN:HB2	4:D:304:EDO:H21	1.98	0.46
3:F:540:MET:O	3:F:540:MET:HG3	2.16	0.46
2:B:166:GLN:OE1	4:B:301:EDO:H22	2.15	0.46
1:A:216:LYS:HG3	5:A:437:HOH:O	2.15	0.46
2:B:142:ARG:O	4:B:305:EDO:H22	2.15	0.46
2:B:143:GLU:HB2	4:B:308:EDO:O2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:TRP:CZ3	2:D:88:CYS:HB3	2.51	0.46
3:E:572:ASP:OD1	3:E:619:THR:HB	2.15	0.46
3:F:639:PRO:HD3	3:F:716:ASN:OD1	2.14	0.46
2:B:12:SER:CB	2:B:105:GLU:OE2	2.63	0.46
3:F:617:VAL:O	3:F:617:VAL:HG13	2.16	0.46
3:E:638:LEU:HD22	3:E:720:SER:O	2.16	0.45
3:F:555:SER:OG	3:F:558:THR:HB	2.16	0.45
3:E:732:LEU:HB3	3:E:733:PRO:HD2	1.98	0.45
1:A:65:MET:HB3	1:A:65:MET:HE2	1.84	0.45
2:B:66:ARG:HG2	2:B:67:SER:N	2.29	0.45
1:A:162:THR:HG23	1:A:163:SER:N	2.31	0.45
3:E:657:ILE:HG21	3:E:672:ILE:HD13	1.98	0.45
1:A:40:ARG:HH12	4:A:302:EDO:H22	1.82	0.45
3:F:732:LEU:HB3	3:F:733:PRO:HD2	1.98	0.45
1:A:63:LYS:HE3	1:A:63:LYS:HB2	1.85	0.44
1:C:60:LEU:HD12	1:C:61:ASN:N	2.32	0.44
2:D:112:ALA:O	4:D:304:EDO:H22	2.17	0.44
1:C:141:GLY:HA2	1:C:156:TRP:CH2	2.52	0.44
3:E:668:SER:HB3	5:E:914:HOH:O	2.16	0.44
2:D:137:ASN:O	4:D:304:EDO:H21	2.18	0.44
2:B:50:ALA:O	2:B:51:THR:HB	2.18	0.44
2:B:173:TYR:OH	4:B:311:EDO:H11	2.17	0.44
2:D:21:LEU:HD22	2:D:102:THR:HG21	1.99	0.44
1:A:201:ASN:HD21	1:A:203:LYS:HE3	1.83	0.44
2:B:46:ARG:H	4:B:307:EDO:C2	2.31	0.44
2:B:46:ARG:H	4:B:307:EDO:H22	1.83	0.44
1:C:40:ARG:HD3	5:C:546:HOH:O	2.17	0.43
3:E:560:ASN:ND2	3:E:600:VAL:O	2.50	0.43
3:F:591:ILE:HD12	3:F:591:ILE:N	2.33	0.43
3:E:549:LEU:CD2	3:E:561:LEU:HD11	2.39	0.43
3:F:638:LEU:N	3:F:638:LEU:HD22	2.32	0.43
1:A:62:GLN:OE1	1:A:65:MET:HG3	2.18	0.43
1:C:150:GLU:HB3	1:C:151:PRO:HA	2.00	0.43
1:C:200:VAL:HB	1:C:209:VAL:CG1	2.48	0.43
2:D:106:ILE:CD1	4:D:301:EDO:H21	2.47	0.43
2:D:188:LYS:HG2	2:D:188:LYS:O	2.18	0.43
3:E:637:ILE:CG2	3:E:638:LEU:N	2.82	0.43
1:A:102:GLY:HA3	4:A:303:EDO:H21	2.01	0.43
3:F:575:TYR:CD2	3:F:592:LYS:HB3	2.53	0.43
3:F:629:LEU:HD22	3:F:629:LEU:N	2.34	0.43
1:A:174:SER:H	4:A:307:EDO:C1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:671:THR:HA	3:F:687:VAL:O	2.18	0.43
3:E:567:PHE:CZ	3:E:569:SER:HB2	2.54	0.43
1:C:202:HIS:O	1:C:206:ASN:N	2.51	0.42
3:E:547:ARG:CG	3:E:548:GLY:N	2.80	0.42
3:E:717:ASN:ND2	3:E:718:ILE:HG12	2.34	0.42
3:F:704:PRO:HG3	3:F:734:GLU:CG	2.49	0.42
2:B:22:THR:HA	2:B:71:TYR:O	2.19	0.42
1:C:205:SER:O	4:C:303:EDO:H11	2.19	0.42
3:E:616:ARG:CD	3:E:623:GLY:O	2.67	0.42
4:B:310:EDO:H22	5:B:453:HOH:O	2.19	0.42
1:C:114:SER:HB2	4:C:306:EDO:C2	2.50	0.42
1:C:148:PHE:HA	1:C:149:PRO:HA	1.81	0.42
3:E:550:ASN:O	3:E:561:LEU:HD12	2.20	0.42
3:F:550:ASN:OD1	3:F:552:LEU:HG	2.18	0.42
2:B:126:LYS:HB3	2:B:126:LYS:HE3	1.80	0.42
3:E:580:ARG:HD2	3:E:580:ARG:C	2.38	0.42
3:F:657:ILE:O	3:F:696:GLN:HA	2.20	0.42
1:C:102:GLY:HA3	4:C:301:EDO:C1	2.42	0.42
3:F:607:PRO:HB2	3:F:636:ASP:HB3	2.01	0.42
1:C:34:MET:O	1:C:50:MET:HA	2.20	0.42
3:E:597:LEU:HD13	3:E:597:LEU:HA	1.85	0.42
3:F:555:SER:HA	3:F:634:LEU:HD12	2.01	0.42
1:C:105:TRP:CZ2	4:C:301:EDO:H12	2.55	0.41
2:D:33:LEU:HA	2:D:89:LEU:O	2.20	0.41
3:E:620:LYS:N	3:E:621:ALA:CA	2.68	0.41
2:D:119:PRO:HB3	2:D:209:PHE:CE1	2.55	0.41
3:E:616:ARG:HD2	3:E:623:GLY:O	2.20	0.41
1:A:40:ARG:HH22	4:A:302:EDO:C2	2.33	0.41
2:B:181:LEU:HA	4:B:310:EDO:H22	2.02	0.41
3:E:575:TYR:CG	3:E:592:LYS:HD2	2.55	0.41
3:E:598:THR:OG1	3:E:598:THR:O	2.39	0.41
1:A:50:MET:HE3	1:A:59:ARG:HG3	2.03	0.41
2:B:85:ASP:OD1	2:B:103:LYS:HG3	2.21	0.41
2:B:107:LYS:HB3	2:B:107:LYS:HE2	1.81	0.41
2:B:129:THR:HG22	2:B:130:ALA:N	2.36	0.41
2:D:26:SER:O	2:D:27:GLN:HG2	2.21	0.41
2:B:46:ARG:HB3	4:B:307:EDO:H11	2.03	0.41
1:C:57:GLU:OE1	3:F:646:LYS:NZ	2.39	0.41
3:F:550:ASN:O	3:F:561:LEU:HD12	2.21	0.41
2:B:143:GLU:H	4:B:308:EDO:C2	2.30	0.40
1:C:203:LYS:C	1:C:206:ASN:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:557:THR:HG22	3:E:605:LEU:H	1.86	0.40
3:E:567:PHE:HD1	3:E:568:PRO:HD2	1.85	0.40
3:F:647:ILE:HG13	3:F:657:ILE:HD12	2.02	0.40
3:F:704:PRO:HG3	3:F:734:GLU:HG3	2.03	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	216/227 (95%)	211 (98%)	5 (2%)	0	100	100
1	C	216/227 (95%)	210 (97%)	6 (3%)	0	100	100
2	B	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
2	D	212/214 (99%)	206 (97%)	5 (2%)	1 (0%)	29	26
3	E	194/199 (98%)	181 (93%)	13 (7%)	0	100	100
3	F	194/199 (98%)	177 (91%)	17 (9%)	0	100	100
All	All	1244/1280 (97%)	1193 (96%)	50 (4%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	28	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/195 (95%)	185 (100%)	1 (0%)	88	92
1	C	186/195 (95%)	185 (100%)	1 (0%)	88	92
2	B	190/190 (100%)	188 (99%)	2 (1%)	73	79
2	D	190/190 (100%)	188 (99%)	2 (1%)	73	79
3	E	175/182 (96%)	173 (99%)	2 (1%)	73	79
3	F	175/182 (96%)	172 (98%)	3 (2%)	60	67
All	All	1102/1134 (97%)	1091 (99%)	11 (1%)	76	82

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	CYS
2	B	56	SER
2	B	93	SER
1	C	98	ARG
2	D	152	ASN
2	D	214	CYS
3	E	540	MET
3	E	599	SER
3	F	547	ARG
3	F	567	PHE
3	F	573	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	137	ASN
2	B	138	ASN
1	C	201	ASN
2	D	138	ASN
3	E	560	ASN
3	E	722	ASN
3	F	560	ASN

5.3.3 RNA ⓘ

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](#)

34 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	$\# Z > 2$
4	EDO	C	303	-	3,3,3	0.51	0	2,2,2	0.16	0
4	EDO	B	302	-	3,3,3	0.47	0	2,2,2	0.29	0
4	EDO	A	306	-	3,3,3	0.59	0	2,2,2	0.13	0
4	EDO	E	801	-	3,3,3	0.47	0	2,2,2	0.35	0
4	EDO	A	305	-	3,3,3	0.53	0	2,2,2	0.17	0
4	EDO	B	308	-	3,3,3	0.63	0	2,2,2	0.33	0
4	EDO	D	305	-	3,3,3	0.43	0	2,2,2	0.54	0
4	EDO	B	303	-	3,3,3	0.50	0	2,2,2	0.37	0
4	EDO	C	301	-	3,3,3	0.34	0	2,2,2	0.26	0
4	EDO	A	301	-	3,3,3	0.53	0	2,2,2	0.31	0
4	EDO	B	304	-	3,3,3	0.51	0	2,2,2	0.30	0
4	EDO	C	305	-	3,3,3	0.49	0	2,2,2	0.27	0
4	EDO	B	311	-	3,3,3	0.60	0	2,2,2	0.15	0
4	EDO	A	308	-	3,3,3	0.56	0	2,2,2	0.29	0
4	EDO	B	309	-	3,3,3	0.49	0	2,2,2	0.20	0
4	EDO	D	304	-	3,3,3	0.50	0	2,2,2	0.16	0
4	EDO	B	301	-	3,3,3	0.61	0	2,2,2	0.16	0
4	EDO	A	309	-	3,3,3	0.50	0	2,2,2	0.16	0
4	EDO	F	801	-	3,3,3	0.54	0	2,2,2	0.15	0
4	EDO	A	302	-	3,3,3	0.51	0	2,2,2	0.30	0
4	EDO	C	306	-	3,3,3	0.52	0	2,2,2	0.07	0
4	EDO	D	302	-	3,3,3	0.56	0	2,2,2	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	306	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	B	307	-	3,3,3	0.44	0	2,2,2	0.61	0
4	EDO	A	307	-	3,3,3	0.52	0	2,2,2	0.27	0
4	EDO	A	303	-	3,3,3	0.49	0	2,2,2	0.40	0
4	EDO	B	305	-	3,3,3	0.50	0	2,2,2	0.25	0
4	EDO	D	303	-	3,3,3	0.61	0	2,2,2	0.22	0
4	EDO	C	304	-	3,3,3	0.52	0	2,2,2	0.17	0
4	EDO	D	301	-	3,3,3	0.50	0	2,2,2	0.27	0
4	EDO	C	302	-	3,3,3	0.46	0	2,2,2	0.35	0
4	EDO	B	310	-	3,3,3	0.50	0	2,2,2	0.37	0
4	EDO	A	310	-	3,3,3	0.49	0	2,2,2	0.33	0
4	EDO	A	304	-	3,3,3	0.56	0	2,2,2	0.30	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	C	303	-	-	0/1/1/1	-
4	EDO	B	302	-	-	1/1/1/1	-
4	EDO	A	306	-	-	1/1/1/1	-
4	EDO	E	801	-	-	0/1/1/1	-
4	EDO	A	305	-	-	0/1/1/1	-
4	EDO	B	308	-	-	1/1/1/1	-
4	EDO	D	305	-	-	0/1/1/1	-
4	EDO	B	303	-	-	0/1/1/1	-
4	EDO	C	301	-	-	0/1/1/1	-
4	EDO	A	301	-	-	1/1/1/1	-
4	EDO	B	304	-	-	0/1/1/1	-
4	EDO	C	305	-	-	0/1/1/1	-
4	EDO	B	311	-	-	1/1/1/1	-
4	EDO	A	308	-	-	0/1/1/1	-
4	EDO	B	309	-	-	0/1/1/1	-
4	EDO	D	304	-	-	1/1/1/1	-
4	EDO	B	301	-	-	1/1/1/1	-
4	EDO	A	309	-	-	0/1/1/1	-
4	EDO	F	801	-	-	0/1/1/1	-
4	EDO	A	302	-	-	1/1/1/1	-
4	EDO	C	306	-	-	1/1/1/1	-
4	EDO	D	302	-	-	1/1/1/1	-
4	EDO	B	306	-	-	1/1/1/1	-
4	EDO	B	307	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	307	-	-	0/1/1/1	-
4	EDO	A	303	-	-	0/1/1/1	-
4	EDO	B	305	-	-	0/1/1/1	-
4	EDO	D	303	-	-	0/1/1/1	-
4	EDO	C	304	-	-	0/1/1/1	-
4	EDO	D	301	-	-	1/1/1/1	-
4	EDO	C	302	-	-	1/1/1/1	-
4	EDO	B	310	-	-	0/1/1/1	-
4	EDO	A	310	-	-	1/1/1/1	-
4	EDO	A	304	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	EDO	O1-C1-C2-O2
4	B	308	EDO	O1-C1-C2-O2
4	C	306	EDO	O1-C1-C2-O2
4	D	302	EDO	O1-C1-C2-O2
4	D	304	EDO	O1-C1-C2-O2
4	B	306	EDO	O1-C1-C2-O2
4	B	311	EDO	O1-C1-C2-O2
4	A	310	EDO	O1-C1-C2-O2
4	A	306	EDO	O1-C1-C2-O2
4	B	302	EDO	O1-C1-C2-O2
4	D	301	EDO	O1-C1-C2-O2
4	B	301	EDO	O1-C1-C2-O2
4	C	302	EDO	O1-C1-C2-O2
4	A	301	EDO	O1-C1-C2-O2

There are no ring outliers.

21 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	303	EDO	1	0
4	B	302	EDO	1	0
4	B	308	EDO	5	0
4	C	301	EDO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	311	EDO	2	0
4	A	308	EDO	1	0
4	D	304	EDO	3	0
4	B	301	EDO	1	0
4	A	309	EDO	1	0
4	F	801	EDO	1	0
4	A	302	EDO	2	0
4	C	306	EDO	4	0
4	D	302	EDO	1	0
4	B	307	EDO	4	0
4	A	307	EDO	2	0
4	A	303	EDO	2	0
4	B	305	EDO	2	0
4	C	304	EDO	2	0
4	D	301	EDO	2	0
4	C	302	EDO	1	0
4	B	310	EDO	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	218/227 (96%)	-0.14	2 (0%) 84 86	14, 28, 52, 90	0
1	C	218/227 (96%)	-0.16	3 (1%) 75 78	15, 28, 50, 90	0
2	B	214/214 (100%)	-0.22	1 (0%) 91 92	14, 26, 43, 71	0
2	D	214/214 (100%)	-0.24	1 (0%) 91 92	14, 26, 43, 83	0
3	E	196/199 (98%)	1.31	53 (27%) 0 0	31, 61, 116, 127	0
3	F	196/199 (98%)	0.80	32 (16%) 1 2	26, 56, 90, 113	0
All	All	1256/1280 (98%)	0.20	92 (7%) 15 19	14, 33, 83, 127	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	574	PHE	8.9
1	A	218	CYS	8.2
3	E	575	TYR	8.1
3	E	567	PHE	8.1
3	E	566	ILE	7.1
3	E	540	MET	6.7
3	E	541	ILE	6.5
3	F	565	PRO	6.5
3	E	570	SER	6.2
3	E	545	PRO	5.7
2	D	214	CYS	5.7
3	E	568	PRO	5.7
3	E	571	GLU	5.6
3	F	567	PHE	5.5
3	F	680	ASN	5.4
3	E	591	ILE	5.2
3	E	621	ALA	5.2
3	E	617	VAL	5.2
3	F	574	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
3	E	594	PRO	5.0
1	C	218	CYS	4.9
3	E	542	GLY	4.9
3	E	598	THR	4.9
3	E	576	VAL	4.9
3	E	596	ASN	4.9
3	E	619	THR	4.8
3	E	544	PRO	4.5
3	E	550	ASN	4.5
3	E	573	ASP	4.5
3	E	572	ASP	4.4
3	E	563	TRP	4.4
3	F	594	PRO	4.3
3	F	591	ILE	4.3
3	E	593	VAL	4.1
3	F	572	ASP	4.0
3	E	595	GLY	4.0
3	E	569	SER	3.9
3	F	540	MET	3.8
3	E	620	LYS	3.8
3	F	566	ILE	3.7
3	E	549	LEU	3.7
3	F	559	LEU	3.7
3	E	601	LEU	3.7
3	E	590	ASN	3.6
3	F	547	ARG	3.6
3	E	552	LEU	3.5
3	F	568	PRO	3.5
3	E	547	ARG	3.5
3	E	597	LEU	3.5
3	F	549	LEU	3.5
3	F	597	LEU	3.5
3	E	622	GLN	3.4
3	E	618	ASN	3.3
3	E	543	LEU	3.2
3	E	548	GLY	3.1
1	A	135	GLY	3.1
3	F	573	ASP	3.1
3	E	623	GLY	3.0
3	F	569	SER	3.0
3	F	557	THR	3.0
3	F	571	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
3	E	564	GLN	2.9
3	E	600	VAL	2.8
3	F	602	LEU	2.8
3	F	605	LEU	2.8
3	E	604	ASN	2.7
3	F	585	LYS	2.7
3	F	679	LYS	2.7
3	F	563	TRP	2.6
3	E	599	SER	2.6
3	E	629	LEU	2.5
2	B	214	CYS	2.5
3	F	678	GLY	2.5
3	E	565	PRO	2.4
3	E	546	PRO	2.4
3	E	602	LEU	2.4
3	E	578	VAL	2.4
3	F	578	VAL	2.4
1	C	192	GLY	2.3
3	F	606	HIS	2.3
3	E	615	ALA	2.3
3	E	613	VAL	2.2
1	C	134	SER	2.2
3	F	682	ASP	2.2
3	F	575	TYR	2.1
3	F	596	ASN	2.1
3	E	559	LEU	2.1
3	F	617	VAL	2.1
3	E	692	ALA	2.1
3	F	586	SER	2.0
3	E	592	LYS	2.0
3	F	583	VAL	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 ⓘ

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	A	302	4/4	0.80	0.20	45,55,62,62	0
4	EDO	C	303	4/4	0.81	0.17	31,53,63,68	0
4	EDO	B	301	4/4	0.83	0.14	30,42,51,51	0
4	EDO	B	311	4/4	0.84	0.24	33,57,65,72	0
4	EDO	B	308	4/4	0.85	0.18	20,38,46,54	0
4	EDO	A	301	4/4	0.87	0.10	35,50,58,60	0
4	EDO	A	306	4/4	0.87	0.16	37,45,50,50	0
4	EDO	D	305	4/4	0.88	0.18	41,49,55,55	0
4	EDO	B	304	4/4	0.89	0.12	50,60,63,65	0
4	EDO	B	307	4/4	0.90	0.26	29,42,50,50	0
4	EDO	A	310	4/4	0.90	0.27	36,44,56,56	0
4	EDO	B	309	4/4	0.90	0.30	43,52,57,61	0
4	EDO	A	304	4/4	0.91	0.12	37,44,51,51	0
4	EDO	A	309	4/4	0.91	0.24	32,55,63,66	0
4	EDO	D	303	4/4	0.91	0.15	28,38,41,48	0
4	EDO	B	310	4/4	0.91	0.27	42,53,56,67	0
4	EDO	C	304	4/4	0.92	0.16	31,42,54,54	0
4	EDO	D	301	4/4	0.92	0.13	36,47,51,59	0
4	EDO	D	302	4/4	0.92	0.13	37,45,52,54	0
4	EDO	C	302	4/4	0.92	0.15	36,43,52,52	0
4	EDO	C	301	4/4	0.92	0.14	30,36,41,41	0
4	EDO	F	801	4/4	0.92	0.10	39,47,55,55	0
4	EDO	B	302	4/4	0.93	0.24	39,49,57,64	0
4	EDO	A	308	4/4	0.94	0.18	39,47,55,56	0
4	EDO	C	305	4/4	0.94	0.22	46,56,63,72	0
4	EDO	C	306	4/4	0.94	0.20	32,39,43,46	0
4	EDO	B	305	4/4	0.94	0.15	33,41,49,58	0
4	EDO	D	304	4/4	0.95	0.19	14,30,37,45	0
4	EDO	B	306	4/4	0.96	0.13	22,45,63,76	0
4	EDO	E	801	4/4	0.96	0.10	33,39,44,48	0
4	EDO	A	307	4/4	0.96	0.14	29,41,49,49	0
4	EDO	B	303	4/4	0.97	0.10	26,37,46,51	0
4	EDO	A	303	4/4	0.97	0.13	30,37,41,44	0
4	EDO	A	305	4/4	0.98	0.12	16,35,41,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.