



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:59 AM UTC

PDB ID : 4AYE / pdb_00004aye
Title : Structure of a complex between CCPs 6 and 7 of Human Complement Factor H and Neisseria meningitidis FHbp Variant 1 E283AE304A mutant
Authors : Johnson, S.; Tan, L.; van der Veen, S.; Caesar, J.; Goicoechea De Jorge, E.; Everett, R.J.; Bai, X.; Exley, R.M.; Ward, P.N.; Ruivo, N.; Trivedi, K.; Cumber, E.; Jones, R.; Newham, L.; Staunton, D.; Borrow, R.; Pickering, M.; Lea, S.M.; Tang, C.M.
Deposited on : 2012-06-20
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

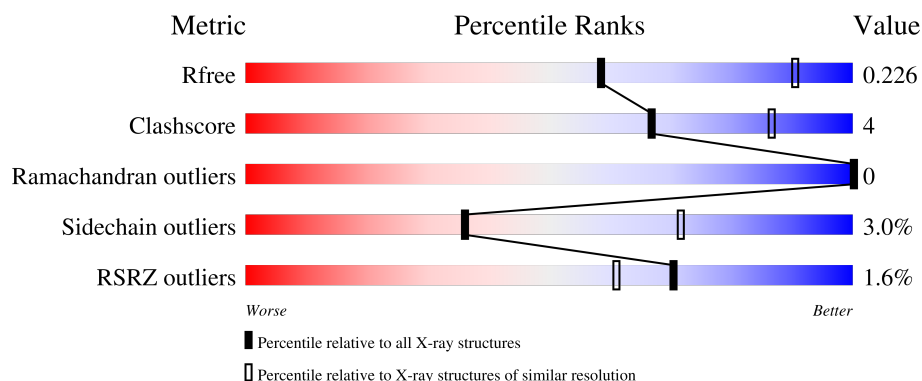
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	125	 2% 85% 12% . .
1	B	125	 % 79% 16% . .
1	E	125	 2% 86% 10% . .
2	C	257	 2% 83% 9% 5%

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	D	257	% 84% 9% • 5%
2	F	257	2% 84% 9% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8654 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 COMPLEMENT FACTOR H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	0	0	0
			999	639	171	179	10			
1	B	120	Total	C	N	O	S	0	0	0
			975	623	167	175	10			
1	E	120	Total	C	N	O	S	0	0	0
			975	623	167	175	10			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	319	MET	-	expression tag	UNP P08603
A	320	GLY	-	expression tag	UNP P08603
A	402	HIS	TYR	variant	UNP P08603
B	319	MET	-	expression tag	UNP P08603
B	320	GLY	-	expression tag	UNP P08603
B	402	HIS	TYR	variant	UNP P08603
E	319	MET	-	expression tag	UNP P08603
E	320	GLY	-	expression tag	UNP P08603
E	402	HIS	TYR	variant	UNP P08603

- Molecule 2 is a protein called FACTOR H BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	243	Total	C	N	O	S	0	0	0
			1832	1139	330	362	1			
2	D	243	Total	C	N	O	S	0	1	0
			1839	1144	332	362	1			
2	F	242	Total	C	N	O	S	0	0	0
			1824	1133	329	361	1			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	72	MET	-	expression tag	UNP Q9JXV4
C	283	ALA	GLU	engineered mutation	UNP Q9JXV4
C	304	ALA	GLU	engineered mutation	UNP Q9JXV4
C	321	GLU	-	expression tag	UNP Q9JXV4
C	322	LEU	-	expression tag	UNP Q9JXV4
C	323	HIS	-	expression tag	UNP Q9JXV4
C	324	HIS	-	expression tag	UNP Q9JXV4
C	325	HIS	-	expression tag	UNP Q9JXV4
C	326	HIS	-	expression tag	UNP Q9JXV4
C	327	HIS	-	expression tag	UNP Q9JXV4
C	328	HIS	-	expression tag	UNP Q9JXV4
D	72	MET	-	expression tag	UNP Q9JXV4
D	283	ALA	GLU	engineered mutation	UNP Q9JXV4
D	304	ALA	GLU	engineered mutation	UNP Q9JXV4
D	321	GLU	-	expression tag	UNP Q9JXV4
D	322	LEU	-	expression tag	UNP Q9JXV4
D	323	HIS	-	expression tag	UNP Q9JXV4
D	324	HIS	-	expression tag	UNP Q9JXV4
D	325	HIS	-	expression tag	UNP Q9JXV4
D	326	HIS	-	expression tag	UNP Q9JXV4
D	327	HIS	-	expression tag	UNP Q9JXV4
D	328	HIS	-	expression tag	UNP Q9JXV4
F	72	MET	-	expression tag	UNP Q9JXV4
F	283	ALA	GLU	engineered mutation	UNP Q9JXV4
F	304	ALA	GLU	engineered mutation	UNP Q9JXV4
F	321	GLU	-	expression tag	UNP Q9JXV4
F	322	LEU	-	expression tag	UNP Q9JXV4
F	323	HIS	-	expression tag	UNP Q9JXV4
F	324	HIS	-	expression tag	UNP Q9JXV4
F	325	HIS	-	expression tag	UNP Q9JXV4
F	326	HIS	-	expression tag	UNP Q9JXV4
F	327	HIS	-	expression tag	UNP Q9JXV4
F	328	HIS	-	expression tag	UNP Q9JXV4

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

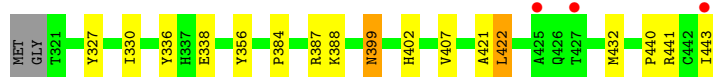
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	11	Total O 11 11	0	0
4	B	18	Total O 18 18	0	0
4	C	41	Total O 41 41	0	0
4	D	24	Total O 24 24	0	0
4	E	21	Total O 21 21	0	0
4	F	19	Total O 19 19	0	0

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.

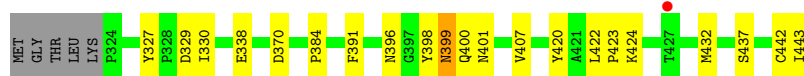
- Molecule 1: COMPLEMENT FACTOR H

Chain A: 



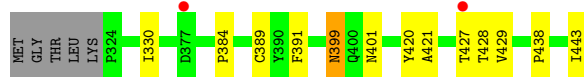
- Molecule 1: COMPLEMENT FACTOR H

Chain B: 



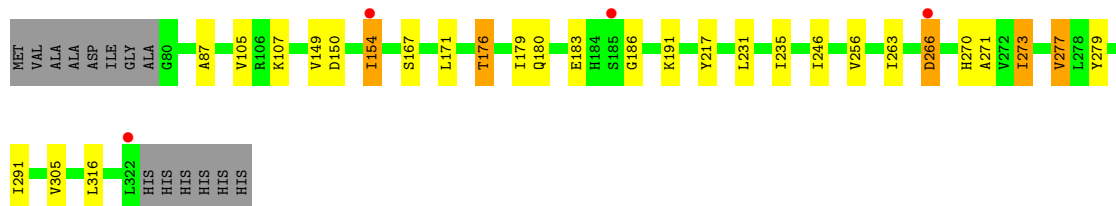
- Molecule 1: COMPLEMENT FACTOR H

Chain E: 



- Molecule 2: FACTOR H BINDING PROTEIN

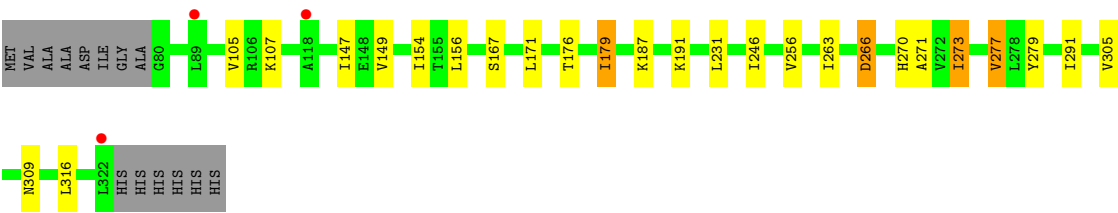
Chain C: 



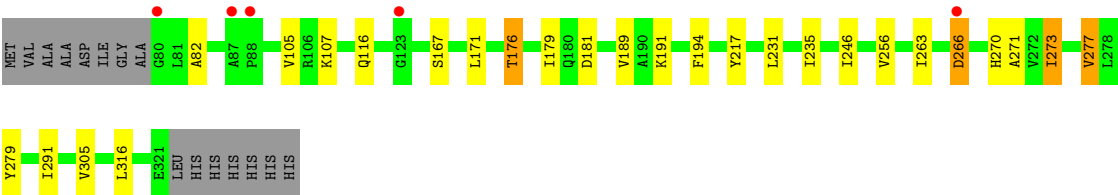
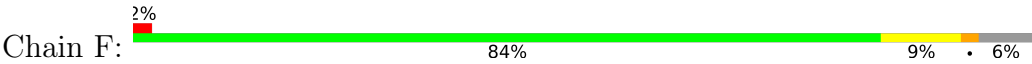
- Molecule 2: FACTOR H BINDING PROTEIN

Chain D: 





● Molecule 2: FACTOR H BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	187.41Å 53.28Å 130.08Å 90.00° 117.74° 90.00°	Depositor
Resolution (Å)	57.57 – 2.80 57.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.3 (57.57-2.80) 93.8 (57.57-2.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.207 , 0.226 0.211 , 0.226	Depositor DCC
R_{free} test set	1347 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8654	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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	0.64	0/1039	1.06	1/1417 (0.1%)
1	B	0.65	0/1015	1.10	2/1384 (0.1%)
1	E	0.66	0/1015	1.12	1/1384 (0.1%)
2	C	0.63	0/1857	1.18	4/2492 (0.2%)
2	D	0.65	0/1868	1.19	3/2507 (0.1%)
2	F	0.65	0/1849	1.20	4/2481 (0.2%)
All	All	0.65	0/8643	1.16	15/11665 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	87	ALA	N-CA-C	6.63	117.22	109.60
1	B	399	ASN	N-CA-C	6.51	120.47	111.55
2	F	181	ASP	CA-CB-CG	5.78	118.38	112.60
2	D	107	LYS	N-CA-C	5.70	120.72	111.37
2	F	266	ASP	CA-CB-CG	5.63	118.23	112.60
2	D	266	ASP	CA-CB-CG	5.59	118.19	112.60
2	C	266	ASP	CA-CB-CG	5.56	118.16	112.60
2	C	107	LYS	N-CA-C	5.54	120.46	111.37
1	B	329	ASP	CA-CB-CG	5.33	117.93	112.60
2	D	167	SER	N-CA-C	5.33	117.09	111.28
2	F	107	LYS	N-CA-C	-5.25	102.27	110.10
2	F	167	SER	N-CA-C	5.20	116.94	111.28
1	E	399	ASN	N-CA-C	5.18	119.30	112.25
1	A	399	ASN	N-CA-C	5.11	118.55	111.55
2	C	167	SER	N-CA-C	5.07	116.80	111.28

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	999	0	915	8	0
1	B	975	0	885	10	0
1	E	975	0	885	8	0
2	C	1832	0	1829	13	0
2	D	1839	0	1836	12	0
2	F	1824	0	1818	13	0
3	A	20	0	30	1	0
3	B	16	0	24	2	0
3	C	12	0	18	0	0
3	D	8	0	12	0	0
3	E	16	0	24	2	0
3	F	4	0	6	1	0
4	A	11	0	0	0	0
4	B	18	0	0	0	0
4	C	41	0	0	0	0
4	D	24	0	0	0	0
4	E	21	0	0	0	0
4	F	19	0	0	0	0
All	All	8654	0	8282	62	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 (62) 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:E:399:ASN:HA	3:E:1447:EDO:H11	1.52	0.89
2:F:194:PHE:HB3	3:F:1322:EDO:H11	1.66	0.77
1:E:421:ALA:H	1:E:443:ILE:HG23	1.56	0.71
2:C:150:ASP:HB3	2:D:309:ASN:HD21	1.58	0.67
1:E:391:PHE:HB3	1:E:401:ASN:O	1.96	0.65
1:E:420:TYR:HD1	1:E:443:ILE:HG12	1.64	0.63
3:A:1445:EDO:H12	1:B:396:ASN:HD22	1.65	0.61
2:D:266:ASP:HB3	2:D:270:HIS:H	1.66	0.60
2:F:266:ASP:HB3	2:F:270:HIS:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:TYR:HB3	1:B:400:GLN:HE22	1.67	0.59
2:C:266:ASP:HB3	2:C:270:HIS:H	1.66	0.59
2:C:179:ILE:HD12	2:C:191:LYS:HB3	1.83	0.59
2:F:256:VAL:HG12	2:F:279:TYR:HB2	1.85	0.58
2:D:277:VAL:HG11	2:D:305:VAL:HG22	1.91	0.53
2:C:277:VAL:HG11	2:C:305:VAL:HG22	1.90	0.53
1:E:420:TYR:CD1	1:E:443:ILE:HG12	2.43	0.53
2:F:277:VAL:HG11	2:F:305:VAL:HG22	1.91	0.53
2:C:176:THR:HG21	2:C:179:ILE:HG12	1.92	0.51
2:D:256:VAL:HG12	2:D:279:TYR:HB2	1.92	0.51
1:E:389:CYS:HA	3:E:1445:EDO:H11	1.93	0.51
2:F:176:THR:HG21	2:F:179:ILE:HG12	1.93	0.50
2:D:149:VAL:HB	2:D:154:ILE:HD12	1.94	0.50
1:B:432:MET:HG3	1:B:437:SER:HB3	1.94	0.49
1:A:330:ILE:HG23	1:A:384:PRO:HG2	1.94	0.49
2:F:179:ILE:HD12	2:F:191:LYS:HD2	1.95	0.48
2:D:147:ILE:HG12	2:D:156:LEU:HG	1.95	0.47
1:A:327:TYR:OH	1:A:338:GLU:HG3	2.16	0.46
1:A:421:ALA:H	1:A:443:ILE:HG12	1.81	0.46
1:B:370:ASP:HA	3:B:1446:EDO:H11	1.98	0.46
2:C:149:VAL:HB	2:C:154:ILE:HD12	1.98	0.45
1:A:422:LEU:HD12	1:A:441:ARG:O	2.16	0.45
1:B:327:TYR:OH	1:B:338:GLU:HG3	2.16	0.45
1:B:399:ASN:HA	3:B:1447:EDO:H12	1.98	0.45
1:B:423:PRO:HA	1:B:424:LYS:HA	1.69	0.45
1:B:420:TYR:HB3	1:B:442:CYS:HB3	1.99	0.45
2:C:231:LEU:HD13	2:C:316:LEU:HD22	1.99	0.45
1:A:387:ARG:HG2	1:A:432:MET:O	2.17	0.44
1:B:391:PHE:HB3	1:B:401:ASN:O	2.18	0.44
2:D:271:ALA:HB1	2:D:291:ILE:HD12	2.00	0.44
2:D:263:ILE:HG12	2:D:273:ILE:HG12	1.98	0.43
2:D:231:LEU:HD13	2:D:316:LEU:HD22	2.00	0.43
2:F:263:ILE:HG12	2:F:273:ILE:HG12	1.99	0.43
2:F:231:LEU:HD13	2:F:316:LEU:HD22	1.99	0.43
2:C:263:ILE:HG12	2:C:273:ILE:HG12	2.00	0.43
2:F:271:ALA:HB1	2:F:291:ILE:HD12	2.01	0.42
2:C:271:ALA:HB1	2:C:291:ILE:HD12	2.01	0.42
2:D:179:ILE:HG12	2:D:191:LYS:HB3	2.02	0.42
2:D:187:LYS:HG3	2:F:189:VAL:HG13	2.02	0.42
1:B:330:ILE:HG23	1:B:384:PRO:HG2	2.02	0.42
2:C:246:ILE:HD11	2:C:316:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LEU:HD11	1:A:440:PRO:HA	2.02	0.42
2:C:180:GLN:HE21	2:C:186:GLY:H	1.67	0.41
2:F:217:TYR:CE1	2:F:235:ILE:HD12	2.55	0.41
1:A:336:TYR:CZ	1:A:356:TYR:HB3	2.55	0.41
2:D:246:ILE:HD11	2:D:316:LEU:HD21	2.02	0.41
1:A:399:ASN:HB3	1:A:402:HIS:HB2	2.02	0.41
2:C:256:VAL:HG12	2:C:279:TYR:HB2	2.03	0.41
1:E:330:ILE:HG23	1:E:384:PRO:HG2	2.02	0.41
2:F:82:ALA:HB2	2:F:116:GLN:HB2	2.03	0.41
2:C:217:TYR:CE1	2:C:235:ILE:HD12	2.56	0.40
2:F:246:ILE:HD11	2:F:316:LEU:HD21	2.03	0.40
1:E:429:VAL:HA	1:E:438:PRO:HD2	2.04	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	121/125 (97%)	114 (94%)	7 (6%)	0	100	100
1	B	118/125 (94%)	109 (92%)	9 (8%)	0	100	100
1	E	118/125 (94%)	110 (93%)	8 (7%)	0	100	100
2	C	241/257 (94%)	233 (97%)	8 (3%)	0	100	100
2	D	242/257 (94%)	237 (98%)	5 (2%)	0	100	100
2	F	240/257 (93%)	233 (97%)	7 (3%)	0	100	100
All	All	1080/1146 (94%)	1036 (96%)	44 (4%)	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	108/109 (99%)	105 (97%)	3 (3%)	38	73
1	B	105/109 (96%)	102 (97%)	3 (3%)	37	73
1	E	105/109 (96%)	103 (98%)	2 (2%)	50	81
2	C	188/198 (95%)	181 (96%)	7 (4%)	30	65
2	D	189/198 (96%)	183 (97%)	6 (3%)	34	70
2	F	187/198 (94%)	182 (97%)	5 (3%)	39	74
All	All	882/921 (96%)	856 (97%)	26 (3%)	36	73

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	388	LYS
1	A	407	VAL
1	A	422	LEU
1	B	407	VAL
1	B	422	LEU
1	B	443	ILE
2	C	105	VAL
2	C	154	ILE
2	C	171	LEU
2	C	176	THR
2	C	183	GLU
2	C	273	ILE
2	C	277	VAL
2	D	105	VAL
2	D	171	LEU
2	D	176	THR
2	D	179	ILE
2	D	273	ILE
2	D	277	VAL
1	E	427	THR
1	E	428	THR
2	F	105	VAL

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Mol	Chain	Res	Type
2	F	171	LEU
2	F	176	THR
2	F	273	ILE
2	F	277	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	HIS
1	A	400	GLN
1	A	401	ASN
1	A	417	HIS
1	B	339	ASN
1	B	396	ASN
1	B	400	GLN
1	B	408	GLN
1	B	417	HIS
2	C	152	GLN
2	C	166	GLN
2	C	180	GLN
2	C	184	HIS
2	C	320	GLN
2	D	91	HIS
2	D	166	GLN
2	D	248	HIS
2	D	281	GLN
2	D	309	ASN
1	E	339	ASN
2	F	91	HIS
2	F	166	GLN
2	F	309	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	B	1444	-	3,3,3	0.55	0	2,2,2	0.32	0
3	EDO	D	1323	-	3,3,3	0.51	0	2,2,2	0.42	0
3	EDO	A	1447	-	3,3,3	0.50	0	2,2,2	0.41	0
3	EDO	B	1445	-	3,3,3	0.55	0	2,2,2	0.27	0
3	EDO	E	1447	-	3,3,3	0.49	0	2,2,2	0.25	0
3	EDO	E	1445	-	3,3,3	0.46	0	2,2,2	0.44	0
3	EDO	F	1322	-	3,3,3	0.54	0	2,2,2	0.23	0
3	EDO	C	1325	-	3,3,3	0.54	0	2,2,2	0.31	0
3	EDO	B	1446	-	3,3,3	0.55	0	2,2,2	0.25	0
3	EDO	E	1444	-	3,3,3	0.52	0	2,2,2	0.34	0
3	EDO	A	1445	-	3,3,3	0.59	0	2,2,2	0.05	0
3	EDO	C	1323	-	3,3,3	0.56	0	2,2,2	0.16	0
3	EDO	D	1324	-	3,3,3	0.52	0	2,2,2	0.37	0
3	EDO	B	1447	-	3,3,3	0.56	0	2,2,2	0.09	0
3	EDO	C	1324	-	3,3,3	0.54	0	2,2,2	0.31	0
3	EDO	A	1446	-	3,3,3	0.55	0	2,2,2	0.26	0
3	EDO	A	1448	-	3,3,3	0.52	0	2,2,2	0.35	0
3	EDO	E	1446	-	3,3,3	0.57	0	2,2,2	0.30	0
3	EDO	A	1444	-	3,3,3	0.55	0	2,2,2	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	1444	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	1323	-	-	0/1/1/1	-
3	EDO	A	1447	-	-	1/1/1/1	-
3	EDO	B	1445	-	-	0/1/1/1	-
3	EDO	E	1447	-	-	1/1/1/1	-
3	EDO	E	1445	-	-	0/1/1/1	-
3	EDO	F	1322	-	-	0/1/1/1	-
3	EDO	C	1325	-	-	1/1/1/1	-
3	EDO	B	1446	-	-	0/1/1/1	-
3	EDO	E	1444	-	-	1/1/1/1	-
3	EDO	A	1445	-	-	0/1/1/1	-
3	EDO	C	1323	-	-	0/1/1/1	-
3	EDO	D	1324	-	-	0/1/1/1	-
3	EDO	B	1447	-	-	0/1/1/1	-
3	EDO	C	1324	-	-	0/1/1/1	-
3	EDO	A	1446	-	-	0/1/1/1	-
3	EDO	A	1448	-	-	0/1/1/1	-
3	EDO	E	1446	-	-	0/1/1/1	-
3	EDO	A	1444	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1444	EDO	O1-C1-C2-O2
3	A	1447	EDO	O1-C1-C2-O2
3	C	1325	EDO	O1-C1-C2-O2
3	A	1444	EDO	O1-C1-C2-O2
3	E	1447	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1447	EDO	1	0
3	E	1445	EDO	1	0
3	F	1322	EDO	1	0
3	B	1446	EDO	1	0
3	A	1445	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1447	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, 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	123/125 (98%)	0.25	3 (2%) 59 49	29, 45, 66, 80	0
1	B	120/125 (96%)	0.13	1 (0%) 82 75	29, 43, 68, 87	0
1	E	120/125 (96%)	-0.13	2 (1%) 69 60	27, 37, 56, 69	0
2	C	243/257 (94%)	0.02	4 (1%) 70 61	24, 38, 71, 94	0
2	D	243/257 (94%)	0.31	3 (1%) 76 68	28, 47, 73, 88	1 (0%)
2	F	242/257 (94%)	0.54	5 (2%) 63 54	28, 50, 74, 96	0
All	All	1091/1146 (95%)	0.22	18 (1%) 70 61	24, 44, 72, 96	1 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	427	THR	3.1
2	F	87	ALA	2.9
2	C	266	ASP	2.6
2	C	185	SER	2.5
2	D	89	LEU	2.4
1	A	443	ILE	2.4
2	C	322	LEU	2.4
2	F	88	PRO	2.4
2	F	80	GLY	2.3
2	D	118	ALA	2.2
2	D	322	LEU	2.2
2	F	123	GLY	2.1
1	A	427	THR	2.1
1	E	427	THR	2.1
1	A	425	ALA	2.1
2	C	154	ILE	2.1
2	F	266	ASP	2.1
1	E	377	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	1446	4/4	0.57	0.20	70,70,70,71	0
3	EDO	D	1323	4/4	0.63	0.15	59,59,59,59	0
3	EDO	F	1322	4/4	0.68	0.27	61,62,63,63	0
3	EDO	B	1445	4/4	0.72	0.21	55,56,58,58	0
3	EDO	E	1446	4/4	0.74	0.17	55,57,58,58	0
3	EDO	A	1445	4/4	0.80	0.21	53,54,55,55	0
3	EDO	A	1448	4/4	0.82	0.13	62,62,63,63	0
3	EDO	C	1324	4/4	0.83	0.21	71,72,72,72	0
3	EDO	C	1325	4/4	0.84	0.16	60,60,60,61	0
3	EDO	A	1444	4/4	0.84	0.19	69,69,69,69	0
3	EDO	A	1447	4/4	0.86	0.16	55,55,55,56	0
3	EDO	E	1445	4/4	0.86	0.19	55,55,57,57	0
3	EDO	C	1323	4/4	0.88	0.19	56,58,59,60	0
3	EDO	E	1447	4/4	0.89	0.24	84,84,85,86	0
3	EDO	B	1447	4/4	0.89	0.14	52,53,54,54	0
3	EDO	B	1444	4/4	0.90	0.18	52,52,53,53	0
3	EDO	D	1324	4/4	0.90	0.16	63,64,64,64	0
3	EDO	E	1444	4/4	0.91	0.13	42,43,44,44	0
3	EDO	B	1446	4/4	0.93	0.11	41,42,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.