WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:31 AM GMT

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PDB ID	:	3EYM
Title	:	Structure of Influenza Haemagglutinin in complex with an inhibitor of membrane fusion
Authors	:	Russell, R.J.; Kerry, P.S.; Stevens, D.A.; Steinhauer, D.A.; Martin, S.R.; Gamblin, S.J.; Skehel, J.J.
Deposited on	:	2008-10-21
Resolution	:	2.80 Å(reported)

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.
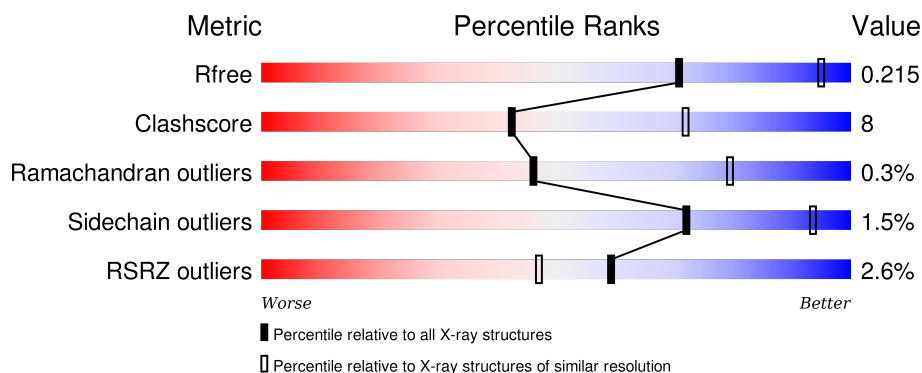
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	321	
1	C	321	
1	E	321	
2	B	172	
2	D	172	

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Mol	Chain	Length	Quality of chain
2	F	172	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11580 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total 2446	C 1532	N 429	O 472	S 13	0	0	0
1	C	318	Total 2455	C 1538	N 431	O 473	S 13	0	0	0
1	E	318	Total 2455	C 1538	N 431	O 473	S 13	0	0	0

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total 1399	C 868	N 246	O 279	S 6	0	0	0
2	D	172	Total 1390	C 868	N 246	O 270	S 6	0	0	0
2	F	172	Total 1399	C 868	N 246	O 279	S 6	0	0	0

- Molecule 3 is 2-TERT-BUTYLBENZENE-1,4-DIOL (three-letter code: EYK) (formula: $C_{10}H_{14}O_2$).
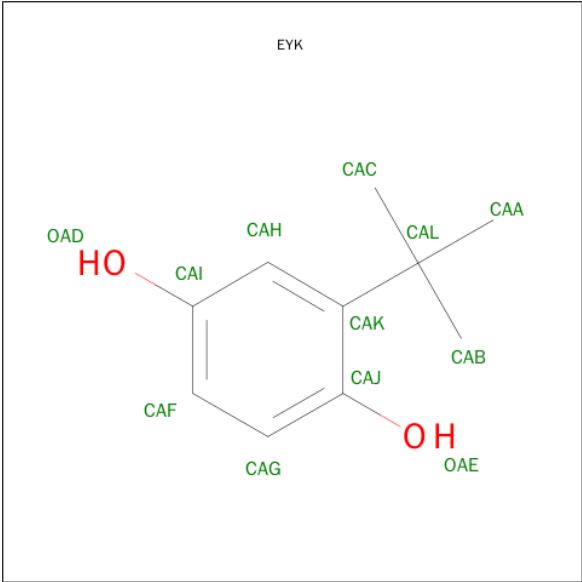
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total 12	C 10	O 2	0	0
3	D	1	Total 12	C 10	O 2	0	0
3	D	1	Total 12	C 10	O 2	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Hemagglutinin HA1 chain
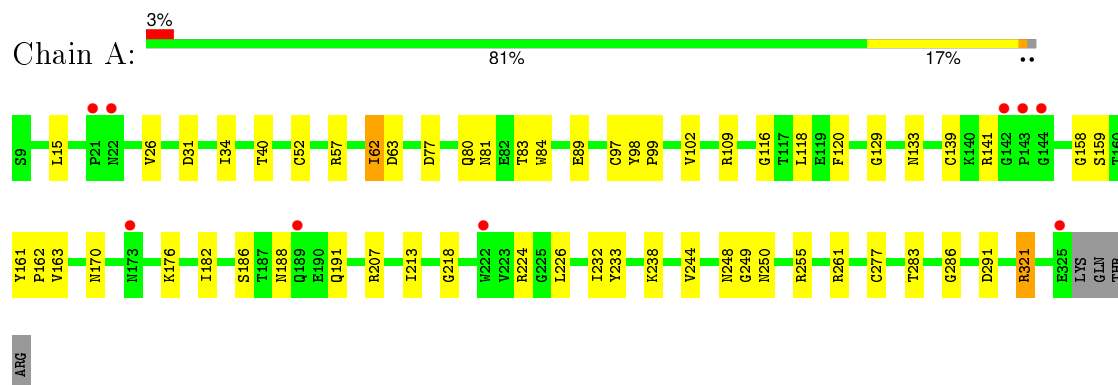
• Molecule 1: Hemagglutinin HA1 chain
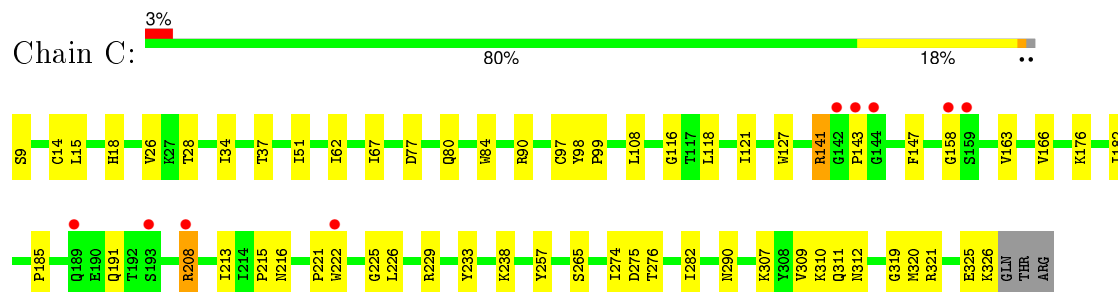
• Molecule 1: Hemagglutinin HA1 chain

• Molecule 2: Hemagglutinin HA2 chain

G1 L2 I18 Q27 N28 S29 T32 K51 I56 E57 K58 S71 N104 Q105 H106 T107 L110 F119 Q125 E131 E132 M133 G134 K139 I140 Y141 H142 E150 R153 N154 G155 Y162 N168 N169 R170 F171 Q172

• Molecule 2: Hemagglutinin HA2 chain

Chain D:

2%
80% 20%

G1 L2 F3 G4 A5 I10 W14 M17 I18 E30 L52 N53 R54 V55 I56 E57 K58 T59 N60 D90 Q105 F119 E120 R123 R124 Q125 L126 R127 E128 E132 M133 G134 N135 K139 I140 Y141 N146 E150 G155 D160 N168 N169 R170 F171

Q172

• Molecule 2: Hemagglutinin HA2 chain

Chain F:

2%
85% 13%

G1 L2 F3 M17 I18 D19 G20 R25 Q34 R54 V55 I56 E57 K58 T59 N60 E74 Q78 S113 L118 F119 R124 E128 E131 E132 E150 R153 R163 L167 R170 F171 Q172

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	160.47Å 160.46Å 176.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.80 19.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.93-2.80) 100.0 (19.93-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.217 0.205 , 0.215	Depositor DCC
R_{free} test set	5462 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	62.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 34.3	EDS
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 109352 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11580	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

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	2/2502 (0.1%)	0.68	2/3410 (0.1%)
1	C	0.66	4/2511 (0.2%)	0.68	0/3421
1	E	0.63	1/2511 (0.0%)	0.69	1/3421 (0.0%)
2	B	0.76	2/1423 (0.1%)	0.71	2/1912 (0.1%)
2	D	0.72	0/1414	0.79	0/1894
2	F	0.70	2/1423 (0.1%)	0.74	0/1912
All	All	0.67	11/11784 (0.1%)	0.71	5/15970 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	58	LYS	CE-NZ	13.52	1.82	1.49
1	C	9	SER	CB-OG	9.31	1.54	1.42
2	B	58	LYS	CD-CE	7.72	1.70	1.51
1	E	158	GLY	C-O	7.07	1.34	1.23
1	A	321	ARG	CZ-NH2	7.06	1.42	1.33
1	C	158	GLY	C-O	5.64	1.32	1.23
2	F	57	GLU	CG-CD	5.47	1.60	1.51
2	F	132	GLU	CG-CD	-5.30	1.44	1.51
1	C	14	CYS	CB-SG	-5.24	1.73	1.81
1	A	238	LYS	CD-CE	5.10	1.64	1.51
1	C	208	ARG	CZ-NH2	5.04	1.39	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ARG	NE-CZ-NH1	-7.90	116.35	120.30
2	B	58	LYS	CD-CE-NZ	-7.53	94.38	111.70
1	E	321	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	A	321	ARG	NE-CZ-NH2	6.22	123.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	110	LEU	CB-CG-CD2	-5.71	101.29	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2446	0	2397	33	0
1	C	2455	0	2410	55	0
1	E	2455	0	2410	41	0
2	B	1399	0	1319	26	0
2	D	1390	0	1319	34	0
2	F	1399	0	1319	24	0
3	D	24	0	27	2	0
3	F	12	0	12	1	0
All	All	11580	0	11213	188	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 8.

All (188) 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:B:58:LYS:NZ	2:B:58:LYS:CE	1.82	1.39
1:C:208:ARG:NH2	1:C:238:LYS:HE3	1.58	1.15
1:C:208:ARG:HH22	1:C:238:LYS:HE3	1.09	1.01
2:D:128:GLU:HG3	2:D:170:ARG:HH11	1.33	0.94
1:C:216:ASN:ND2	1:E:212:THR:OG1	2.01	0.94
1:C:99:PRO:CD	1:C:226:LEU:HD12	2.00	0.90
1:E:63:ASP:OD1	1:E:92:LYS:HG3	1.74	0.87
2:D:30:GLU:OE1	2:D:146:ASN:CG	2.14	0.84
1:C:182:ILE:HD11	1:C:215:PRO:HD3	1.61	0.81
1:C:99:PRO:HD3	1:C:226:LEU:HD12	1.63	0.80
1:C:221:PRO:O	1:C:229:ARG:NH1	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:GLU:HG2	2:B:134:GLY:H	1.46	0.78
2:D:128:GLU:HG3	2:D:170:ARG:NH1	2.00	0.76
1:E:283:THR:OG1	1:E:286:GLY:O	2.05	0.74
1:E:99:PRO:CD	1:E:226:LEU:HD12	2.19	0.73
1:E:230:ILE:HD13	1:E:252:ILE:HG13	1.70	0.73
1:E:99:PRO:HD3	1:E:226:LEU:HD12	1.72	0.70
1:A:98:TYR:CD2	1:A:99:PRO:HD2	2.27	0.69
1:A:283:THR:OG1	1:A:286:GLY:O	2.09	0.69
3:F:173:EYK:OAE	3:F:173:EYK:HAC	1.93	0.69
1:E:309:VAL:HG13	1:E:311:GLN:OE1	1.93	0.68
1:C:77:ASP:O	1:C:80:GLN:HG3	1.95	0.66
2:B:58:LYS:NZ	2:B:58:LYS:CD	2.59	0.66
2:B:132:GLU:HG2	2:B:134:GLY:N	2.12	0.65
2:D:30:GLU:OE1	2:D:146:ASN:ND2	2.30	0.65
1:C:141:ARG:NH1	1:C:147:PHE:O	2.31	0.63
2:B:150:GLU:HG2	2:B:153:ARG:NH2	2.12	0.63
1:C:99:PRO:HD2	1:C:226:LEU:HD12	1.79	0.63
2:B:132:GLU:CG	2:B:134:GLY:H	2.12	0.63
1:C:307:LYS:HE3	2:D:60:ASN:HD21	1.64	0.63
1:A:182:ILE:HD13	1:A:213:ILE:HG22	1.82	0.62
2:D:5:ALA:O	2:D:10:ILE:HB	2.01	0.61
1:A:84:TRP:HZ3	1:A:118:LEU:HG	1.65	0.61
1:C:275:ASP:OD2	1:C:276:THR:N	2.33	0.61
1:C:222:TRP:CZ2	1:C:225:GLY:HA2	2.37	0.60
1:C:77:ASP:OD1	1:C:141:ARG:NH2	2.35	0.59
2:B:150:GLU:HG2	2:B:153:ARG:HH22	1.67	0.59
1:C:216:ASN:CG	1:E:212:THR:OG1	2.41	0.59
1:A:158:GLY:O	1:A:159:SER:HB3	2.03	0.59
2:B:56:ILE:O	2:B:56:ILE:HG22	2.03	0.59
2:F:54:ARG:O	2:F:57:GLU:HG2	2.03	0.59
2:D:168:ASN:HA	2:D:172:GLN:OE1	2.03	0.58
2:F:74:GLU:HG3	2:F:78:GLN:NE2	2.18	0.58
1:C:90:ARG:NH1	1:C:274:ILE:HD12	2.18	0.58
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.38	0.58
1:C:208:ARG:CZ	1:C:238:LYS:HG3	2.35	0.57
1:C:325:GLU:O	1:C:326:LYS:HB3	2.03	0.57
1:C:84:TRP:HZ3	1:C:118:LEU:HG	1.69	0.57
1:E:213:ILE:HD12	1:E:213:ILE:N	2.19	0.57
1:A:97:CYS:O	1:A:224:ARG:NH1	2.30	0.57
3:D:174:EYK:HAC	3:D:174:EYK:OAE	2.04	0.56
1:A:77:ASP:O	1:A:80:GLN:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:TRP:HZ3	1:E:118:LEU:HG	1.72	0.55
2:B:168:ASN:ND2	2:B:172:GLN:CG	2.70	0.55
2:D:2:LEU:HB3	2:F:3:PHE:CZ	2.40	0.55
2:D:52:LEU:CD1	2:D:56:ILE:HD12	2.37	0.55
1:C:185:PRO:HG2	1:C:191:GLN:OE1	2.07	0.55
1:A:129:GLY:HA3	1:A:162:PRO:HG3	1.88	0.55
3:D:173:EYK:HAC	3:D:173:EYK:OAE	2.06	0.54
2:F:171:PHE:O	2:F:172:GLN:HB2	2.07	0.54
2:B:125:GLN:OE1	2:B:155:GLY:HA2	2.08	0.54
1:A:207:ARG:HG2	1:E:223:VAL:HG22	1.90	0.54
1:E:77:ASP:OD1	1:E:141:ARG:NH2	2.41	0.54
1:E:23:GLY:HA3	1:E:35:GLU:OE2	2.08	0.54
1:E:77:ASP:O	1:E:80:GLN:HG3	2.08	0.54
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.91	0.53
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.90	0.53
1:C:309:VAL:HG13	1:C:311:GLN:OE1	2.09	0.53
1:A:81:ASN:ND2	1:A:120:PHE:H	2.06	0.53
1:A:81:ASN:HD21	1:A:120:PHE:H	1.56	0.52
1:A:249:GLY:O	1:A:250:ASN:HB2	2.08	0.52
1:C:213:ILE:HG12	1:C:233:TYR:CZ	2.44	0.52
1:A:186:SER:HA	1:A:218:GLY:O	2.09	0.52
2:D:120:GLU:CD	2:D:123:ARG:HH22	2.13	0.52
1:A:31:ASP:OD2	1:A:34:ILE:HD12	2.10	0.52
1:A:84:TRP:CZ3	1:A:118:LEU:HG	2.44	0.52
2:D:52:LEU:HD11	2:D:56:ILE:CD1	2.40	0.52
1:E:51:ILE:HG23	1:E:282:ILE:HD12	1.92	0.51
1:A:52:CYS:HB3	1:A:277:CYS:O	2.10	0.51
1:C:307:LYS:CE	2:D:60:ASN:HD21	2.21	0.51
1:E:307:LYS:NZ	2:F:60:ASN:OD1	2.29	0.51
1:C:163:VAL:HG23	1:C:163:VAL:O	2.11	0.51
1:C:51:ILE:HG23	1:C:282:ILE:HD12	1.91	0.51
1:C:208:ARG:NH2	1:C:238:LYS:CE	2.52	0.51
1:C:99:PRO:HD2	1:C:226:LEU:CD1	2.40	0.51
2:F:150:GLU:OE1	2:F:153:ARG:NH2	2.44	0.50
1:A:98:TYR:CZ	1:A:226:LEU:HD13	2.47	0.50
2:D:56:ILE:HG22	2:D:56:ILE:O	2.11	0.50
1:C:90:ARG:HH12	1:C:274:ILE:HD12	1.77	0.50
1:C:216:ASN:ND2	1:E:203:THR:OG1	2.45	0.50
2:F:54:ARG:HA	2:F:57:GLU:CD	2.31	0.50
1:C:98:TYR:CD2	1:C:99:PRO:HD2	2.46	0.50
2:D:132:GLU:CD	2:F:124:ARG:HE	2.14	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:THR:OG1	1:C:319:GLY:HA3	2.12	0.49
2:F:119:PHE:HZ	2:F:132:GLU:CG	2.25	0.49
1:C:127:TRP:CZ3	1:C:166:VAL:HG21	2.47	0.49
2:D:132:GLU:OE2	2:F:124:ARG:NE	2.42	0.49
2:D:53:ASN:O	2:D:57:GLU:HB2	2.12	0.49
1:C:163:VAL:O	1:C:163:VAL:CG2	2.61	0.49
1:A:133:ASN:OD1	1:A:255:ARG:NH1	2.46	0.49
1:E:98:TYR:CD2	1:E:99:PRO:HD2	2.48	0.49
1:C:26:VAL:HG22	1:C:34:ILE:O	2.12	0.48
2:B:51:LYS:HE3	2:B:107:THR:OG1	2.13	0.48
2:B:27:GLN:HB2	2:B:32:THR:HG22	1.96	0.48
1:C:310:LYS:HE3	2:D:90:ASP:OD2	2.13	0.48
1:C:28:THR:HB	2:D:105:GLN:OE1	2.13	0.48
1:E:151:LEU:O	1:E:255:ARG:NH2	2.46	0.48
2:B:142:HIS:CD2	2:B:162:TYR:HB3	2.49	0.48
2:F:74:GLU:HG3	2:F:78:GLN:HE21	1.77	0.48
2:F:25:ARG:HG3	2:F:34:GLN:HG3	1.96	0.48
2:D:2:LEU:HB3	2:F:3:PHE:HZ	1.79	0.47
2:B:168:ASN:ND2	2:B:172:GLN:HG3	2.29	0.47
2:F:54:ARG:HA	2:F:57:GLU:OE2	2.14	0.47
2:D:132:GLU:HG2	2:D:134:GLY:H	1.80	0.47
1:A:89:GLU:OE2	1:A:109:ARG:NH2	2.48	0.47
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.96	0.47
2:F:17:MET:HE2	2:F:20:GLY:O	2.15	0.47
1:C:320:MET:HG3	1:C:321:ARG:O	2.15	0.47
2:B:139:LYS:HE2	2:B:141:TYR:CE2	2.49	0.47
2:D:56:ILE:CG2	2:D:56:ILE:O	2.63	0.47
1:C:216:ASN:ND2	1:E:212:THR:CB	2.78	0.46
1:A:26:VAL:HG13	2:B:104:ASN:ND2	2.31	0.46
2:D:2:LEU:O	2:F:113:SER:OG	2.32	0.46
1:C:99:PRO:HB2	1:C:229:ARG:HD3	1.97	0.46
1:C:208:ARG:HH22	1:C:238:LYS:CE	2.00	0.46
1:C:176:LYS:HE2	1:C:257:TYR:CE2	2.51	0.46
2:B:2:LEU:HB3	2:D:3:PHE:HZ	1.82	0.45
2:B:2:LEU:HB3	2:D:3:PHE:CZ	2.51	0.45
2:B:58:LYS:HG3	2:B:58:LYS:H	1.62	0.45
2:B:139:LYS:HE2	2:B:141:TYR:CZ	2.52	0.45
1:E:87:PHE:O	1:E:267:ILE:HG13	2.17	0.45
1:E:84:TRP:CE2	1:E:116:GLY:HA2	2.52	0.45
2:D:139:LYS:HD3	2:D:141:TYR:CZ	2.51	0.45
1:E:212:THR:C	1:E:213:ILE:HD12	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:131:GLU:HG3	2:F:170:ARG:HD2	1.98	0.45
1:E:89:GLU:HG3	1:E:267:ILE:HD11	1.97	0.45
1:A:291:ASP:O	2:B:56:ILE:HG23	2.16	0.44
1:E:84:TRP:CZ3	1:E:118:LEU:HG	2.52	0.44
2:F:56:ILE:O	2:F:56:ILE:HG22	2.15	0.44
1:C:325:GLU:O	1:C:326:LYS:CB	2.66	0.44
1:C:127:TRP:CH2	1:C:166:VAL:HG21	2.52	0.44
2:F:17:MET:HE2	2:F:17:MET:HB3	1.78	0.44
2:D:125:GLN:OE1	2:D:155:GLY:HA2	2.17	0.44
1:C:121:ILE:HD12	1:C:257:TYR:CE1	2.52	0.44
1:C:274:ILE:HG22	1:C:275:ASP:N	2.33	0.44
1:E:31:ASP:OD2	1:E:34:ILE:HD12	2.18	0.43
2:B:106:HIS:CE1	2:B:110:LEU:HD23	2.53	0.43
1:E:119:GLU:OE1	1:E:261:ARG:NH2	2.50	0.43
2:F:171:PHE:O	2:F:172:GLN:CB	2.65	0.43
2:D:135:ASN:OD1	2:D:135:ASN:N	2.52	0.43
1:C:15:LEU:HD22	2:D:119:PHE:HA	2.00	0.43
1:E:176:LYS:HE2	1:E:257:TYR:CE2	2.53	0.43
1:E:97:CYS:O	1:E:224:ARG:NH1	2.45	0.43
2:D:30:GLU:OE1	2:D:146:ASN:CB	2.67	0.43
1:E:15:LEU:HD22	2:F:119:PHE:HA	2.00	0.43
1:E:310:LYS:HB2	1:E:310:LYS:HE3	1.79	0.43
1:A:188:ASN:HA	1:A:191:GLN:HB3	2.00	0.43
1:A:161:TYR:HA	1:A:162:PRO:HD2	1.86	0.43
1:C:84:TRP:CZ3	1:C:118:LEU:HG	2.51	0.43
1:A:163:VAL:HG22	1:A:248:ASN:HB3	2.01	0.43
1:A:57:ARG:HD3	1:A:83:THR:O	2.19	0.42
1:C:98:TYR:CZ	1:C:226:LEU:HD13	2.53	0.42
2:B:131:GLU:OE1	2:D:127:ARG:NH2	2.50	0.42
1:E:301:THR:HB	1:E:305:CYS:SG	2.59	0.42
1:E:89:GLU:OE2	1:E:109:ARG:NH2	2.51	0.42
1:E:213:ILE:HG12	1:E:233:TYR:CZ	2.54	0.42
1:C:67:ILE:HD12	1:C:108:LEU:HD23	2.01	0.42
1:E:29:ILE:HA	1:E:29:ILE:HD13	1.92	0.42
1:E:71:LEU:O	1:E:148:PHE:HB3	2.19	0.42
1:A:213:ILE:HG12	1:A:233:TYR:CZ	2.55	0.41
1:A:97:CYS:HA	1:A:139:CYS:HB2	2.02	0.41
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.55	0.41
2:F:163:ARG:O	2:F:167:LEU:HG	2.20	0.41
1:C:290:ASN:HB2	2:D:59:THR:HG21	2.03	0.41
1:A:244:VAL:HG23	1:E:221:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:GLU:CD	2:D:124:ARG:HE	2.23	0.41
1:C:221:PRO:HG2	1:E:206:THR:C	2.41	0.41
1:C:90:ARG:NH1	1:C:274:ILE:CD1	2.82	0.41
1:A:62:ILE:HG22	1:A:63:ASP:N	2.36	0.41
1:C:99:PRO:CD	1:C:226:LEU:CD1	2.85	0.40
2:D:132:GLU:CG	2:D:134:GLY:H	2.33	0.40
1:E:15:LEU:HD23	2:F:118:LEU:HG	2.02	0.40
2:F:128:GLU:OE1	2:F:170:ARG:NH1	2.53	0.40
1:C:97:CYS:SG	1:C:98:TYR:N	2.90	0.40
2:B:170:ARG:HG2	2:B:171:PHE:CE1	2.56	0.40
1:E:213:ILE:N	1:E:213:ILE:CD1	2.83	0.40
1:A:170:ASN:HA	1:A:176:LYS:NZ	2.36	0.40
2:D:14:TRP:HE3	2:D:17:MET:HE3	1.87	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	315/321 (98%)	304 (96%)	10 (3%)	1 (0%)	46	79
1	C	316/321 (98%)	296 (94%)	18 (6%)	2 (1%)	30	65
1	E	316/321 (98%)	301 (95%)	14 (4%)	1 (0%)	46	79
2	B	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
2	D	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
2	F	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
All	All	1457/1479 (98%)	1390 (95%)	63 (4%)	4 (0%)	46	79

All (4) Ramachandran outliers are listed below:

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Mol	Chain	Res	Type
1	A	62	ILE
1	E	62	ILE
1	C	62	ILE
1	C	143	PRO

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	279/283 (99%)	275 (99%)	4 (1%)	74	94
1	C	280/283 (99%)	276 (99%)	4 (1%)	74	94
1	E	280/283 (99%)	276 (99%)	4 (1%)	74	94
2	B	147/147 (100%)	145 (99%)	2 (1%)	74	94
2	D	147/147 (100%)	143 (97%)	4 (3%)	52	85
2	F	147/147 (100%)	146 (99%)	1 (1%)	88	97
All	All	1280/1290 (99%)	1261 (98%)	19 (2%)	72	93

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	141	ARG
1	A	261	ARG
1	A	321	ARG
2	B	57	GLU
2	B	58	LYS
1	C	18	HIS
1	C	141	ARG
1	C	265	SER
1	C	312	ASN
2	D	54	ARG
2	D	128	GLU
2	D	150	GLU
2	D	160	ASP
1	E	18	HIS

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Mol	Chain	Res	Type
1	E	215	PRO
1	E	222	TRP
1	E	224	ARG
2	F	132	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	80	GLN
1	A	81	ASN
2	B	168	ASN
1	C	38	ASN
1	C	216	ASN
2	D	60	ASN
2	D	65	GLN
1	E	38	ASN
1	E	165	ASN
1	E	246	ASN
2	F	78	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry (i)

3 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	EYK	D	173	-	12,12,12	1.05	1 (8%)	18,18,18	2.17	8 (44%)
3	EYK	D	174	-	12,12,12	1.30	1 (8%)	18,18,18	2.45	7 (38%)
3	EYK	F	173	-	12,12,12	1.04	1 (8%)	18,18,18	2.14	6 (33%)

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	EYK	D	173	-	-	0/6/6/6	0/1/1/1
3	EYK	D	174	-	-	0/6/6/6	0/1/1/1
3	EYK	F	173	-	-	0/6/6/6	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	173	EYK	CAH-CAI	2.27	1.42	1.39
3	D	173	EYK	CAH-CAI	2.37	1.42	1.39
3	D	174	EYK	CAH-CAI	3.48	1.44	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	174	EYK	CAL-CAK-CAJ	-6.40	118.07	122.31
3	D	173	EYK	CAL-CAK-CAJ	-4.62	119.25	122.31
3	F	173	EYK	CAL-CAK-CAJ	-4.36	119.42	122.31
3	F	173	EYK	CAC-CAL-CAA	-3.35	97.09	108.32
3	F	173	EYK	CAG-CAF-CAI	-3.35	116.00	119.87
3	D	174	EYK	CAC-CAL-CAA	-3.32	97.19	108.32
3	D	173	EYK	CAB-CAL-CAK	-3.17	104.85	110.86
3	D	174	EYK	CAG-CAF-CAI	-3.12	116.26	119.87
3	D	173	EYK	CAG-CAF-CAI	-2.45	117.04	119.87
3	D	173	EYK	CAC-CAL-CAA	-2.40	100.29	108.32
3	D	174	EYK	CAB-CAL-CAK	-2.09	106.90	110.86
3	D	173	EYK	CAF-CAI-CAH	2.04	122.53	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	173	EYK	CAG-CAJ-CAK	2.13	123.01	120.43
3	F	173	EYK	CAH-CAK-CAL	2.20	125.71	120.13
3	D	173	EYK	CAC-CAL-CAK	2.21	115.06	110.86
3	D	174	EYK	CAG-CAJ-CAK	2.30	123.22	120.43
3	D	174	EYK	CAH-CAK-CAL	2.61	126.74	120.13
3	D	173	EYK	CAG-CAJ-CAK	3.33	124.46	120.43
3	D	173	EYK	CAA-CAL-CAK	3.78	118.03	110.86
3	D	174	EYK	CAA-CAL-CAK	4.12	118.67	110.86
3	F	173	EYK	CAA-CAL-CAK	4.43	119.28	110.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	173	EYK	1	0
3	D	174	EYK	1	0
3	F	173	EYK	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(Å²)	Q<0.9
1	A	317/321 (98%)	-0.24	9 (2%)	56	44	40, 56, 81, 89	0
1	C	318/321 (99%)	-0.13	9 (2%)	56	44	41, 61, 81, 91	0
1	E	318/321 (99%)	-0.28	7 (2%)	65	54	38, 54, 69, 84	0
2	B	172/172 (100%)	-0.31	6 (3%)	48	35	36, 57, 79, 91	0
2	D	172/172 (100%)	-0.43	3 (1%)	73	63	35, 51, 70, 90	0
2	F	172/172 (100%)	-0.47	4 (2%)	64	52	36, 52, 70, 89	0
All	All	1469/1479 (99%)	-0.28	38 (2%)	59	47	35, 55, 79, 91	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	143	PRO	4.4
1	C	142	GLY	4.1
1	A	143	PRO	4.1
1	A	222	TRP	4.0
2	F	58	LYS	3.9
2	B	58	LYS	3.6
2	D	58	LYS	3.4
1	A	22	ASN	3.4
2	B	18	ILE	3.3
2	D	57	GLU	3.1
2	B	29	SER	3.1
1	E	22	ASN	3.1
1	C	222	TRP	3.0
1	C	208	ARG	2.8
1	E	143	PRO	2.8
1	A	189	GLN	2.8
1	E	326	LYS	2.8
1	A	173	ASN	2.7
1	E	222	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	142	GLY	2.6
2	B	71	SER	2.6
2	F	60	ASN	2.4
1	E	144	GLY	2.3
2	B	32	THR	2.3
1	A	21	PRO	2.2
1	C	193	SER	2.2
2	D	18	ILE	2.2
2	F	18	ILE	2.2
1	A	325	GLU	2.2
1	C	158	GLY	2.1
1	A	144	GLY	2.1
2	B	172	GLN	2.1
1	E	142	GLY	2.1
1	C	189	GLN	2.1
1	C	159	SER	2.1
2	F	57	GLU	2.0
1	E	173	ASN	2.0
1	C	144	GLY	2.0

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

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

6.3   Carbohydrates (i)

There are no carbohydrates in this entry.

6.4   Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	EYK	F	173	12/12	0.92	0.27	0.54	58,67,70,72	0
3	EYK	D	173	12/12	0.89	0.27	0.34	62,72,77,80	0
3	EYK	D	174	12/12	0.91	0.24	0.24	54,62,66,66	0

6.5 Other polymers (i)

There are no such residues in this entry.