Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 01:51 AM EDT

PDB ID	:	1FX3
Title	:	CRYSTAL STRUCTURE OF H. INFLUENZAE SECB
Authors	:	Xu, Z.; Knafels, J.D.; Yoshino, K.
Deposited on	:	2000-09-25
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

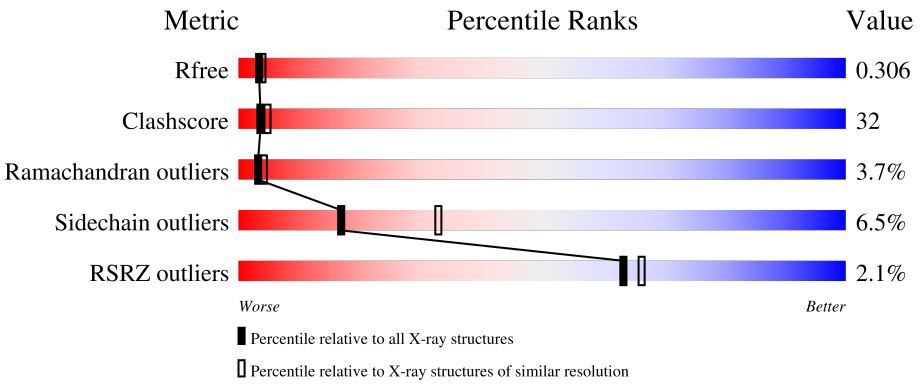
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	169	4%, 38%, 39%, 5%, •, 15%
1	B	169	%, 49%, 36%, •, 12%
1	C	169	46%, 35%, •, 16%
1	D	169	3%, 40%, 34%, 6%, •, 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4485 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 PROTEIN-EXPORT PROTEIN SECB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	143	1098	702	175	215	6	0	0	0
1	B	149	1174	747	190	231	6	0	0	0
1	C	142	1114	713	180	215	6	0	0	0
1	D	135	1036	665	165	200	6	0	0	0

- Molecule 2 is water.

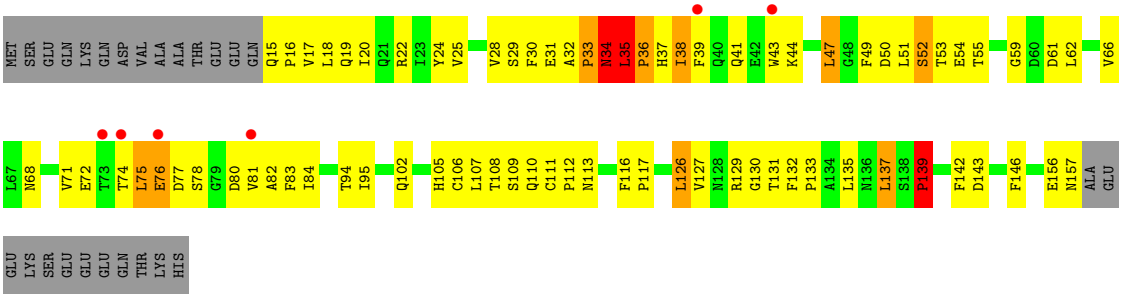
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	15	15	15	0	0
2	B	15	15	15	0	0
2	C	21	21	21	0	0
2	D	12	12	12	0	0

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.

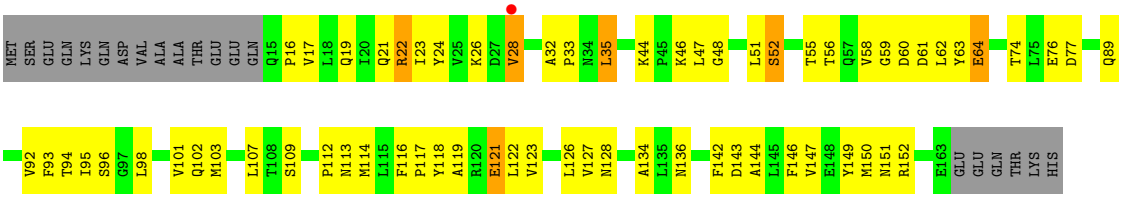
• Molecule 1: PROTEIN-EXPORT PROTEIN SECB

Chain A:



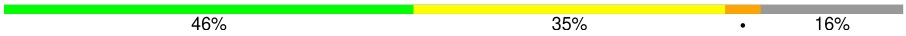
• Molecule 1: PROTEIN-EXPORT PROTEIN SECB

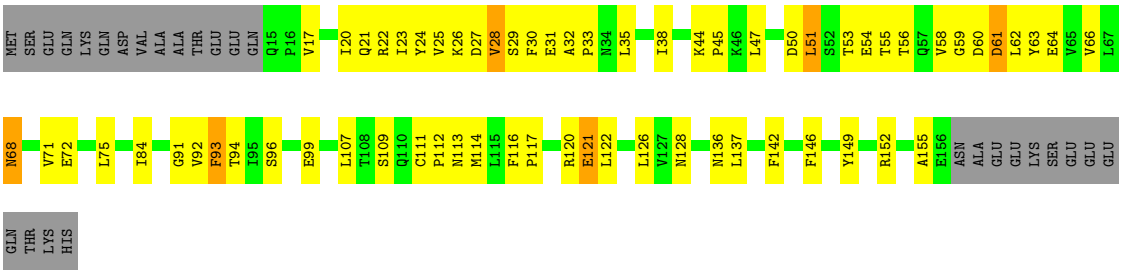
Chain B:



• Molecule 1: PROTEIN-EXPORT PROTEIN SECB

Chain C:

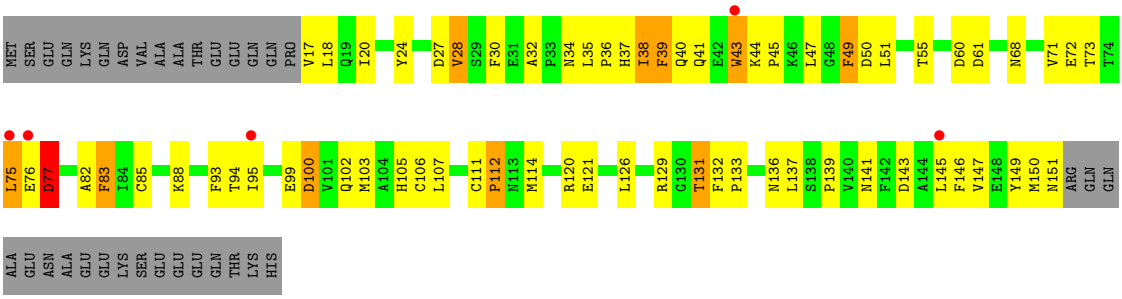




• Molecule 1: PROTEIN-EXPORT PROTEIN SECB

Chain D:

3%
40%
34%
6%
20%


MET SER GLU GLN LYS GLN ASP VAL ALA ALA THR GLU GLU GLN GLN PRO V17 L18 Q19 I20 Y24 D27 V28 S29 F30 E31 A32 P33 N34 L35 P36 H37 I38 F39 Q40 Q41 E42 W43 K44 P45 K46 L47 G48 F49 D50 L51 T55 D60 D61 N68 V71 E72 T73 T74
L75 E76 D77 A82 F83 I84 C85 K88 F93 T94 I95 E99 D100 V101 Q102 M103 A104 H105 C106 L107 C111 P112 N113 M114 R120 E121 L126 R129 G130 T131 F132 P133 N136 L137 S138 P139 V140 N141 F142 D143 A144 L145 F146 V147 E148 Y149 M150 N151 ARG GLN GLN
ALA GLU ASN ALA GLU GLU LYS SER GLU GLU GLU GLN THR LYS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	126.34Å 126.34Å 148.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.95 – 2.50 96.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.3 (44.95-2.50) 98.0 (96.18-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.32 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.301 0.246 , 0.306	Depositor DCC
R_{free} test set	4238 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å^2)	51.8	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 64.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4485	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.58	0/1122	0.80	1/1535 (0.1%)
1	B	0.58	0/1198	0.75	0/1631
1	C	0.61	0/1138	0.80	0/1552
1	D	0.51	0/1058	0.78	0/1447
All	All	0.57	0/4516	0.78	1/6165 (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	A	35	LEU	N-CA-C	5.56	126.01	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	1098	0	1034	77	0
1	B	1174	0	1135	68	0
1	C	1114	0	1080	69	0
1	D	1036	0	992	82	0
2	A	15	0	0	1	0
2	B	15	0	0	1	0
2	C	21	0	0	3	0
2	D	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4485	0	4241	275	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 32.

All (275) 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:A:47:LEU:HD12	1:A:47:LEU:H	1.17	1.08
1:A:19:GLN:HE21	1:A:20:ILE:H	1.07	0.93
1:D:43:TRP:NE1	1:D:133:PRO:HG2	1.87	0.89
1:C:21:GLN:HB2	1:C:92:VAL:HG12	1.55	0.88
1:D:32:ALA:O	1:D:35:LEU:HD23	1.73	0.88
1:A:25:VAL:HG11	1:A:28:VAL:HG23	1.55	0.86
1:C:72:GLU:HG3	1:C:84:ILE:HG12	1.58	0.86
1:C:22:ARG:HG2	1:D:39:PHE:CE1	2.11	0.85
1:A:55:THR:HG21	1:A:107:LEU:HD13	1.56	0.85
1:A:32:ALA:O	1:A:35:LEU:HD23	1.78	0.83
1:A:19:GLN:HE21	1:A:20:ILE:N	1.76	0.83
1:B:51:LEU:HD23	1:B:52:SER:N	1.94	0.83
1:C:68:ASN:HD22	1:C:68:ASN:N	1.76	0.82
1:A:19:GLN:NE2	1:A:20:ILE:H	1.79	0.80
1:D:43:TRP:HA	1:D:43:TRP:CE3	2.15	0.80
1:C:30:PHE:HB3	1:D:28:VAL:HG13	1.64	0.79
1:D:43:TRP:HA	1:D:43:TRP:HE3	1.48	0.78
1:C:58:VAL:HA	2:C:173:HOH:O	1.82	0.78
1:A:43:TRP:NE1	1:A:133:PRO:HG3	1.99	0.77
1:B:26:LYS:NZ	1:B:64:GLU:OE2	2.17	0.76
1:D:55:THR:HG21	1:D:107:LEU:HD13	1.66	0.76
1:B:98:LEU:HD12	1:B:103:MET:HE2	1.69	0.75
1:A:30:PHE:HB3	1:B:28:VAL:HG13	1.70	0.74
1:D:47:LEU:H	1:D:47:LEU:HD12	1.53	0.73
1:A:126:LEU:O	1:A:129:ARG:N	2.20	0.73
1:C:51:LEU:C	1:C:51:LEU:HD12	2.09	0.73
1:C:60:ASP:O	1:C:61:ASP:HB2	1.90	0.71
1:D:49:PHE:HD2	1:D:50:ASP:H	1.38	0.71
1:B:22:ARG:HB3	1:B:22:ARG:HH11	1.54	0.71
1:A:47:LEU:H	1:A:47:LEU:CD1	1.93	0.70
1:C:116:PHE:HB3	1:C:117:PRO:HD3	1.73	0.70
1:A:49:PHE:CD2	1:A:50:ASP:N	2.60	0.70
1:D:18:LEU:O	1:D:18:LEU:HD23	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:HD23	1:A:52:SER:N	2.06	0.69
1:C:66:VAL:HG12	1:C:68:ASN:ND2	2.08	0.69
1:D:34:ASN:HB2	1:D:38:ILE:HD11	1.76	0.68
1:D:41:GLN:HG3	2:D:172:HOH:O	1.94	0.68
1:B:119:ALA:O	1:B:123:VAL:HG23	1.94	0.68
1:B:51:LEU:HD23	1:B:51:LEU:C	2.13	0.68
1:B:146:PHE:O	1:B:149:TYR:HB3	1.94	0.68
1:A:47:LEU:HD12	1:A:47:LEU:N	2.01	0.67
1:D:32:ALA:HB1	1:D:35:LEU:HD21	1.76	0.67
1:D:82:ALA:O	1:D:132:PHE:CZ	2.48	0.67
1:A:33:PRO:O	1:A:35:LEU:N	2.20	0.66
1:B:128:ASN:HD21	1:C:136:ASN:HD21	1.44	0.66
1:C:111:CYS:HB2	1:C:112:PRO:HD3	1.78	0.65
1:D:99:GLU:O	1:D:102:GLN:HG2	1.97	0.65
1:A:18:LEU:HD13	1:A:106:CYS:SG	2.37	0.65
1:D:43:TRP:CD1	1:D:133:PRO:HG2	2.32	0.64
1:A:111:CYS:HB2	1:A:112:PRO:HD3	1.80	0.64
1:A:49:PHE:HE2	1:A:51:LEU:HB2	1.61	0.64
1:C:55:THR:HG21	1:C:107:LEU:HD13	1.80	0.64
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.62	0.63
1:D:18:LEU:HD12	1:D:106:CYS:SG	2.38	0.63
1:B:23:ILE:HD12	1:D:136:ASN:CG	2.19	0.63
1:A:71:VAL:HG11	1:A:135:LEU:HD21	1.78	0.63
1:A:25:VAL:CG1	1:A:28:VAL:HG23	2.28	0.63
1:C:66:VAL:HG12	1:C:68:ASN:HD21	1.63	0.62
1:C:26:LYS:HE3	1:C:64:GLU:OE2	2.00	0.61
1:A:135:LEU:HG	1:A:135:LEU:O	2.01	0.61
1:B:136:ASN:HD21	1:C:128:ASN:HD21	1.48	0.61
1:B:89:GLN:HB2	1:B:119:ALA:HB2	1.82	0.61
1:D:34:ASN:CB	1:D:38:ILE:HD11	2.31	0.61
1:A:31:GLU:HG2	1:A:33:PRO:HD3	1.81	0.60
1:A:113:ASN:HD22	1:A:142:PHE:HD1	1.46	0.60
1:C:59:GLY:HA3	1:C:62:LEU:HB2	1.83	0.60
1:D:76:GLU:O	1:D:77:ASP:HB3	2.01	0.60
1:A:17:VAL:O	1:A:95:ILE:HA	2.01	0.59
1:A:139:PRO:HG3	1:C:114:MET:HE1	1.84	0.59
1:C:27:ASP:OD1	1:C:28:VAL:N	2.34	0.59
1:A:37:HIS:O	1:A:39:PHE:N	2.35	0.59
1:C:121:GLU:OE2	1:D:129:ARG:NH2	2.36	0.59
1:A:25:VAL:HG11	1:A:28:VAL:CG2	2.29	0.59
1:B:55:THR:HG21	1:B:107:LEU:HD13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ASN:O	1:D:38:ILE:HG13	2.02	0.59
1:B:44:LYS:HB3	1:B:76:GLU:HB2	1.84	0.58
1:B:44:LYS:CB	1:B:76:GLU:HB2	2.33	0.58
1:B:61:ASP:O	1:B:94:THR:HA	2.04	0.58
1:B:56:THR:HG22	1:B:58:VAL:HG13	1.85	0.58
1:B:98:LEU:HB2	1:B:103:MET:HE2	1.84	0.58
1:A:82:ALA:O	1:A:132:PHE:CZ	2.57	0.58
1:A:72:GLU:O	1:A:72:GLU:HG2	2.04	0.57
1:B:98:LEU:HB2	1:B:103:MET:CE	2.34	0.57
1:C:22:ARG:HG2	1:D:39:PHE:HE1	1.62	0.57
1:A:24:TYR:CD1	1:B:35:LEU:HD23	2.39	0.56
1:A:35:LEU:O	1:A:37:HIS:N	2.38	0.56
1:B:21:GLN:O	1:B:22:ARG:HG2	2.05	0.56
1:C:120:ARG:HG3	1:C:137:LEU:HB2	1.87	0.56
1:A:143:ASP:O	1:A:146:PHE:HB3	2.06	0.56
1:B:24:TYR:HE2	1:B:92:VAL:HG23	1.71	0.56
1:C:61:ASP:O	1:C:94:THR:HA	2.06	0.56
1:C:113:ASN:HD22	1:C:142:PHE:HD1	1.52	0.55
1:D:43:TRP:HZ3	1:D:75:LEU:CD1	2.20	0.55
1:B:123:VAL:O	1:B:127:VAL:HG13	2.06	0.55
1:A:35:LEU:O	1:A:36:PRO:C	2.44	0.55
1:C:121:GLU:CG	1:D:129:ARG:HH22	2.20	0.55
1:C:59:GLY:CA	1:C:62:LEU:HB2	2.36	0.55
1:D:20:ILE:HG12	1:D:93:PHE:CE2	2.42	0.55
1:C:24:TYR:OH	1:C:64:GLU:HG3	2.07	0.54
1:C:47:LEU:HD11	1:C:71:VAL:HG13	1.88	0.54
1:C:35:LEU:HD12	1:C:38:ILE:CG2	2.37	0.54
1:B:98:LEU:HD12	1:B:103:MET:CE	2.36	0.54
1:D:82:ALA:O	1:D:83:PHE:HB3	2.08	0.54
1:C:68:ASN:N	1:C:68:ASN:ND2	2.46	0.54
1:D:143:ASP:O	1:D:146:PHE:HB3	2.07	0.54
1:D:111:CYS:HB2	1:D:112:PRO:HD3	1.90	0.54
1:A:44:LYS:O	1:A:75:LEU:HA	2.08	0.54
1:C:120:ARG:HD2	1:C:137:LEU:O	2.08	0.53
1:C:60:ASP:O	1:C:61:ASP:CB	2.54	0.53
1:A:61:ASP:O	1:A:94:THR:HA	2.08	0.53
1:D:105:HIS:HE1	1:D:143:ASP:OD1	1.92	0.53
1:D:149:TYR:C	1:D:151:ASN:H	2.12	0.53
1:D:30:PHE:O	1:D:30:PHE:CD2	2.61	0.53
1:D:141:ASN:O	1:D:145:LEU:HG	2.09	0.53
1:C:30:PHE:HB3	1:D:28:VAL:CG1	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:PHE:HB3	1:D:133:PRO:CD	2.39	0.53
1:C:47:LEU:CD1	1:C:71:VAL:HG13	2.39	0.53
1:A:80:ASP:HB2	2:A:180:HOH:O	2.09	0.52
1:C:121:GLU:HG3	1:D:129:ARG:HH22	1.75	0.52
1:A:49:PHE:CE2	1:A:51:LEU:HB2	2.42	0.52
1:C:51:LEU:C	1:C:51:LEU:CD1	2.77	0.52
1:D:126:LEU:O	1:D:129:ARG:N	2.33	0.52
1:D:37:HIS:O	1:D:38:ILE:HG12	2.09	0.52
1:A:82:ALA:O	1:A:83:PHE:HB3	2.10	0.52
1:D:51:LEU:C	1:D:51:LEU:HD23	2.30	0.52
1:D:44:LYS:N	1:D:45:PRO:CD	2.73	0.51
1:C:51:LEU:HD12	1:C:51:LEU:O	2.09	0.51
1:B:60:ASP:O	1:B:61:ASP:HB2	2.10	0.51
1:A:33:PRO:C	1:A:35:LEU:H	2.11	0.51
1:A:35:LEU:HD12	1:B:24:TYR:CE1	2.46	0.51
1:A:129:ARG:HG3	1:A:129:ARG:NH1	2.26	0.51
1:D:18:LEU:CD1	1:D:106:CYS:SG	2.98	0.51
1:C:64:GLU:HA	1:C:91:GLY:O	2.10	0.51
1:D:44:LYS:H	1:D:75:LEU:HD21	1.75	0.51
1:D:83:PHE:CD1	1:D:83:PHE:C	2.84	0.50
1:B:114:MET:HE1	1:D:139:PRO:HG3	1.93	0.50
1:A:156:GLU:O	1:A:157:ASN:C	2.49	0.50
1:C:55:THR:HG22	1:C:56:THR:N	2.26	0.50
1:C:109:SER:O	1:C:112:PRO:HD2	2.12	0.50
1:C:122:LEU:HD11	1:C:126:LEU:HD11	1.94	0.50
1:B:23:ILE:HD12	1:D:136:ASN:OD1	2.12	0.49
1:A:49:PHE:HE1	1:A:137:LEU:HD13	1.77	0.49
1:C:61:ASP:O	1:C:62:LEU:HD22	2.12	0.49
1:B:64:GLU:HB2	1:B:92:VAL:HG22	1.94	0.49
1:B:95:ILE:CD1	1:B:107:LEU:HD21	2.41	0.49
1:A:81:VAL:HG11	1:A:84:ILE:HG13	1.94	0.49
1:C:92:VAL:HG12	1:C:92:VAL:O	2.12	0.49
1:B:150:MET:O	1:B:152:ARG:N	2.46	0.49
1:D:71:VAL:HG23	1:D:71:VAL:O	2.12	0.49
1:B:109:SER:C	1:B:112:PRO:HD2	2.33	0.49
1:D:149:TYR:O	1:D:151:ASN:N	2.46	0.49
1:A:34:ASN:O	1:A:38:ILE:HB	2.13	0.48
1:B:113:ASN:ND2	1:B:142:PHE:CD1	2.78	0.48
1:D:71:VAL:CG2	1:D:85:CYS:HB3	2.43	0.48
1:D:38:ILE:C	1:D:40:GLN:H	2.16	0.48
1:A:49:PHE:HD2	1:A:50:ASP:N	2.08	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLN:O	1:A:105:HIS:N	2.43	0.48
1:C:21:GLN:O	1:C:22:ARG:HB2	2.13	0.48
1:A:28:VAL:CG1	1:A:29:SER:N	2.76	0.48
1:B:35:LEU:CD1	1:B:35:LEU:N	2.77	0.48
1:C:35:LEU:HD12	1:C:38:ILE:HG21	1.95	0.48
1:A:28:VAL:HG12	1:A:29:SER:N	2.29	0.48
1:B:19:GLN:CG	1:B:94:THR:HB	2.44	0.48
1:B:22:ARG:HH11	1:B:22:ARG:CB	2.23	0.48
1:B:46:LYS:HB3	1:B:74:THR:OG1	2.12	0.48
1:C:93:PHE:CD1	1:C:93:PHE:N	2.82	0.48
1:D:38:ILE:C	1:D:40:GLN:N	2.66	0.47
1:D:27:ASP:OD1	1:D:28:VAL:N	2.47	0.47
1:B:63:TYR:CD1	1:B:95:ILE:HD12	2.49	0.47
1:C:24:TYR:HE1	1:C:26:LYS:HG2	1.77	0.47
1:C:99:GLU:OE1	1:C:99:GLU:N	2.36	0.47
1:D:38:ILE:O	1:D:40:GLN:N	2.48	0.47
1:A:19:GLN:NE2	1:A:20:ILE:HG22	2.29	0.47
1:A:51:LEU:HD23	1:A:51:LEU:C	2.33	0.47
1:C:61:ASP:C	1:C:62:LEU:HD22	2.35	0.47
1:D:17:VAL:O	1:D:95:ILE:HA	2.15	0.47
1:D:18:LEU:HA	1:D:94:THR:O	2.15	0.47
1:A:116:PHE:N	1:A:117:PRO:HD2	2.30	0.47
1:C:56:THR:HG22	1:C:58:VAL:HG13	1.96	0.47
1:A:83:PHE:CD1	1:A:83:PHE:C	2.88	0.47
1:B:59:GLY:HA3	1:B:62:LEU:HB2	1.97	0.47
1:B:113:ASN:ND2	1:B:142:PHE:HD1	2.12	0.47
1:C:25:VAL:HG11	1:C:28:VAL:HG12	1.97	0.47
1:C:38:ILE:HD11	1:C:75:LEU:HD12	1.97	0.47
1:C:68:ASN:HD22	1:C:68:ASN:H	1.59	0.47
1:A:132:PHE:HB3	1:A:133:PRO:HD2	1.96	0.47
1:B:114:MET:CE	1:D:139:PRO:HG3	2.45	0.47
1:B:35:LEU:HB2	2:B:172:HOH:O	2.16	0.46
1:B:101:VAL:HG13	1:B:102:GLN:N	2.31	0.46
1:D:68:ASN:HD22	1:D:88:LYS:HG2	1.81	0.46
1:D:82:ALA:O	1:D:132:PHE:HZ	1.93	0.46
1:D:76:GLU:O	1:D:77:ASP:CB	2.64	0.46
1:A:59:GLY:H	1:A:62:LEU:HB2	1.80	0.46
1:A:108:THR:HG22	1:A:108:THR:O	2.16	0.46
1:B:21:GLN:HB2	1:B:92:VAL:O	2.16	0.46
1:B:143:ASP:O	1:B:146:PHE:HB3	2.15	0.46
1:D:111:CYS:O	1:D:114:MET:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:PHE:O	1:C:149:TYR:HB3	2.15	0.46
1:D:72:GLU:HG2	1:D:72:GLU:O	2.16	0.46
1:D:83:PHE:C	1:D:83:PHE:HD1	2.20	0.46
1:B:17:VAL:O	1:B:95:ILE:HA	2.15	0.45
1:B:122:LEU:HD11	1:B:126:LEU:HD11	1.97	0.45
1:C:17:VAL:HB	1:C:96:SER:OG	2.16	0.45
1:B:19:GLN:HG3	1:B:94:THR:HB	1.99	0.45
1:C:44:LYS:NZ	2:C:184:HOH:O	2.48	0.45
1:D:100:ASP:O	1:D:103:MET:HB3	2.16	0.45
1:B:64:GLU:HA	1:B:92:VAL:HA	1.96	0.45
1:D:49:PHE:HD2	1:D:50:ASP:N	2.09	0.45
1:D:43:TRP:NE1	1:D:133:PRO:CG	2.70	0.45
1:A:106:CYS:HA	1:A:110:GLN:HB2	1.99	0.45
1:D:37:HIS:O	1:D:38:ILE:CG1	2.65	0.45
1:B:47:LEU:HD12	1:B:48:GLY:N	2.31	0.45
1:B:109:SER:O	1:B:112:PRO:HD2	2.17	0.45
1:C:20:ILE:HG21	1:C:23:ILE:HD11	1.99	0.45
1:D:147:VAL:C	1:D:149:TYR:H	2.21	0.45
1:A:71:VAL:HG11	1:A:135:LEU:CD2	2.46	0.44
1:A:15:GLN:HA	1:A:16:PRO:HD3	1.84	0.44
1:B:51:LEU:C	1:B:51:LEU:CD2	2.85	0.44
1:C:31:GLU:HG2	1:C:33:PRO:HD3	1.98	0.44
1:C:35:LEU:HD23	1:D:24:TYR:CD1	2.52	0.44
1:A:53:THR:HA	1:A:66:VAL:O	2.17	0.44
1:D:151:ASN:N	1:D:151:ASN:ND2	2.64	0.44
1:B:16:PRO:HA	1:B:96:SER:O	2.17	0.44
1:B:23:ILE:HD13	1:B:118:TYR:CZ	2.53	0.44
1:C:53:THR:HG22	1:C:54:GLU:N	2.32	0.44
1:D:149:TYR:C	1:D:151:ASN:N	2.71	0.43
1:C:35:LEU:HD12	1:C:38:ILE:HG22	2.00	0.43
1:A:139:PRO:HG3	1:C:114:MET:CE	2.46	0.43
1:B:121:GLU:HG3	1:B:122:LEU:N	2.32	0.43
1:A:32:ALA:N	1:A:33:PRO:HD3	2.34	0.43
1:A:43:TRP:CD1	1:A:133:PRO:HG3	2.53	0.43
1:B:95:ILE:HD13	1:B:107:LEU:HD21	2.00	0.43
1:D:39:PHE:CZ	1:D:131:THR:HB	2.53	0.43
1:D:61:ASP:O	1:D:94:THR:HA	2.18	0.43
1:C:152:ARG:O	1:C:155:ALA:HB3	2.19	0.42
1:C:92:VAL:HG21	1:D:36:PRO:HG3	2.01	0.42
1:A:32:ALA:HB1	1:A:35:LEU:CD2	2.50	0.42
1:A:135:LEU:O	1:A:135:LEU:CG	2.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:PHE:HB3	1:B:117:PRO:HD3	2.02	0.42
1:C:136:ASN:HA	2:C:172:HOH:O	2.20	0.42
1:A:43:TRP:NE1	1:A:133:PRO:CG	2.77	0.42
1:B:19:GLN:HE21	1:B:21:GLN:NE2	2.17	0.42
1:D:44:LYS:O	1:D:75:LEU:HD23	2.20	0.42
1:B:114:MET:CE	1:D:120:ARG:NH2	2.83	0.42
1:D:34:ASN:HB2	1:D:38:ILE:CD1	2.47	0.41
1:B:24:TYR:HE1	1:B:26:LYS:CG	2.33	0.41
1:B:60:ASP:O	1:B:61:ASP:CB	2.68	0.41
1:C:109:SER:C	1:C:112:PRO:HD2	2.40	0.41
1:D:51:LEU:HA	1:D:68:ASN:O	2.20	0.41
1:A:77:ASP:OD2	1:A:78:SER:N	2.53	0.41
1:C:32:ALA:HA	1:C:33:PRO:HD2	1.81	0.41
1:D:43:TRP:CE2	1:D:133:PRO:HG2	2.53	0.41
1:A:130:GLY:O	1:A:131:THR:OG1	2.35	0.41
1:B:44:LYS:HB2	1:B:76:GLU:HB2	2.02	0.41
1:D:35:LEU:N	1:D:35:LEU:HD22	2.35	0.41
1:D:151:ASN:N	1:D:151:ASN:HD22	2.18	0.41
1:A:43:TRP:CE2	1:A:133:PRO:HG3	2.55	0.41
1:A:126:LEU:HA	1:A:126:LEU:HD23	1.78	0.41
1:A:38:ILE:HD13	1:A:82:ALA:HA	2.02	0.41
1:B:55:THR:HG22	1:B:56:THR:N	2.36	0.41
1:A:19:GLN:HE21	1:A:20:ILE:HG22	1.86	0.41
1:A:72:GLU:O	1:A:72:GLU:CG	2.69	0.41
1:A:109:SER:O	1:A:113:ASN:HB2	2.20	0.41
1:C:26:LYS:CE	1:C:64:GLU:OE2	2.67	0.41
1:D:49:PHE:CE1	1:D:137:LEU:HD22	2.56	0.41
1:B:93:PHE:CD1	1:B:93:PHE:N	2.88	0.40
1:B:32:ALA:HA	1:B:33:PRO:HD2	1.90	0.40
1:B:103:MET:O	1:B:107:LEU:HG	2.21	0.40
1:C:63:TYR:O	1:C:92:VAL:HA	2.22	0.40
1:A:54:GLU:HG3	1:A:68:ASN:HD21	1.86	0.40
1:D:82:ALA:HB1	1:D:132:PHE:HE2	1.86	0.40
1:A:135:LEU:C	1:A:135:LEU:HD12	2.42	0.40
1:B:24:TYR:CE2	1:B:92:VAL:HG23	2.52	0.40
1:B:144:ALA:O	1:B:147:VAL:HB	2.22	0.40
1:D:73:THR:HG22	1:D:82:ALA:HB3	2.04	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	141/169 (83%)	109 (77%)	20 (14%)	12 (8%)	1 1
1	B	147/169 (87%)	132 (90%)	12 (8%)	3 (2%)	7 12
1	C	140/169 (83%)	132 (94%)	7 (5%)	1 (1%)	22 39
1	D	133/169 (79%)	110 (83%)	18 (14%)	5 (4%)	3 4
All	All	561/676 (83%)	483 (86%)	57 (10%)	21 (4%)	3 4

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	PRO
1	A	34	ASN
1	A	38	ILE
1	A	76	GLU
1	D	77	ASP
1	A	75	LEU
1	A	137	LEU
1	B	77	ASP
1	B	151	ASN
1	C	61	ASP
1	D	38	ILE
1	D	100	ASP
1	D	150	MET
1	A	35	LEU
1	B	134	ALA
1	D	39	PHE
1	A	36	PRO
1	A	41	GLN
1	A	126	LEU
1	A	139	PRO
1	A	127	VAL

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	120/152 (79%)	112 (93%)	8 (7%)	16	31
1	B	132/152 (87%)	126 (96%)	6 (4%)	27	51
1	C	125/152 (82%)	117 (94%)	8 (6%)	17	33
1	D	115/152 (76%)	105 (91%)	10 (9%)	10	20
All	All	492/608 (81%)	460 (94%)	32 (6%)	17	33

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	34	ASN
1	A	35	LEU
1	A	47	LEU
1	A	52	SER
1	A	74	THR
1	A	76	GLU
1	A	139	PRO
1	B	22	ARG
1	B	28	VAL
1	B	35	LEU
1	B	52	SER
1	B	64	GLU
1	B	121	GLU
1	C	28	VAL
1	C	29	SER
1	C	45	PRO
1	C	50	ASP
1	C	51	LEU
1	C	68	ASN
1	C	93	PHE
1	C	121	GLU
1	D	28	VAL
1	D	43	TRP

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Mol	Chain	Res	Type
1	D	49	PHE
1	D	60	ASP
1	D	75	LEU
1	D	77	ASP
1	D	83	PHE
1	D	112	PRO
1	D	121	GLU
1	D	131	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	21	GLN
1	A	136	ASN
1	B	21	GLN
1	B	128	ASN
1	B	141	ASN
1	C	41	GLN
1	C	68	ASN
1	C	128	ASN
1	D	41	GLN
1	D	57	GLN
1	D	68	ASN
1	D	105	HIS
1	D	151	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	143/169 (84%)	0.62	6 (4%) 36 39	32, 58, 92, 113	0
1	B	149/169 (88%)	0.53	1 (0%) 87 89	25, 52, 83, 104	0
1	C	142/169 (84%)	0.51	0 100 100	29, 48, 83, 115	0
1	D	135/169 (79%)	0.63	5 (3%) 41 45	38, 63, 102, 118	0
All	All	569/676 (84%)	0.57	12 (2%) 63 66	25, 56, 96, 118	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	75	LEU	4.2
1	A	43	TRP	4.2
1	D	145	LEU	3.9
1	D	43	TRP	3.1
1	A	76	GLU	2.9
1	D	76	GLU	2.8
1	D	95	ILE	2.6
1	A	39	PHE	2.5
1	B	28	VAL	2.1
1	A	81	VAL	2.1
1	A	74	THR	2.1
1	A	73	THR	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.