



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:51 AM UTC

PDB ID : 2H3X / pdb_00002h3x
Title : Crystal Structure of an Electron Transfer Complex Between Aromatic Amine Dehydrogenase and Azurin from *Alcaligenes Faecalis* (Form 3)
Authors : Sukumar, N.; Chen, Z.; Leys, D.; Scrutton, N.S.; Ferrati, D.; Merli, A.; Rossi, G.L.; Bellamy, H.D.; Chistoserdov, A.; Davidson, V.L.; Mathews, F.S.
Deposited on : 2006-05-23
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 ⓘ 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)
Validation Pipeline (wwPDB-VP)	:	2.49

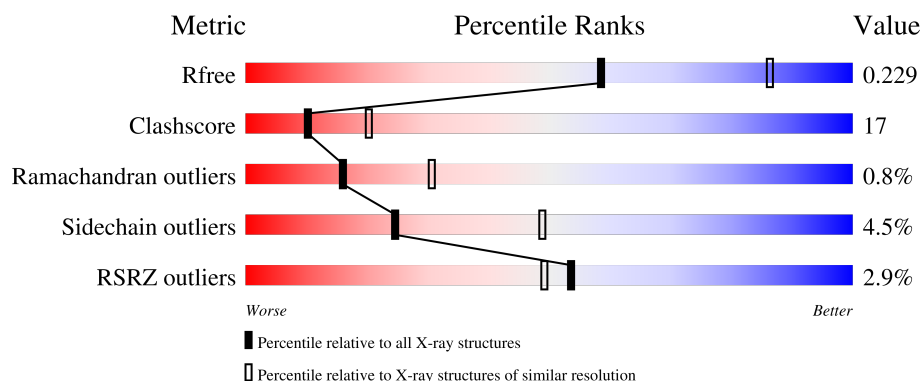
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	390	71% 19% • 8%
1	D	390	% 70% 20% • 8%
2	B	135	% 56% 30% 5% • 7%
2	E	135	55% 31% 5% • 8%
3	C	128	16% 56% 36% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	128	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '8%', followed by a large green segment labeled '55%', then a large yellow segment labeled '38%', and a small orange segment at the end labeled '7%'.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10086 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 Aromatic Amine Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2805	1770	489	533	13			
1	D	359	Total	C	N	O	S	0	0	0
			2805	1770	489	533	13			

- Molecule 2 is a protein called Aromatic Amine Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	125	Total	C	N	O	S	0	0	0
			956	582	168	191	15			
2	E	124	Total	C	N	O	S	0	0	0
			951	579	167	190	15			

- Molecule 3 is a protein called Azurin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	128	Total	C	N	O	S	0	0	0
			958	596	160	195	7			
3	F	128	Total	C	N	O	S	0	0	0
			958	596	160	195	7			

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cu	0	0
			1	1		
4	F	1	Total	Cu	0	0
			1	1		

- Molecule 5 is water.

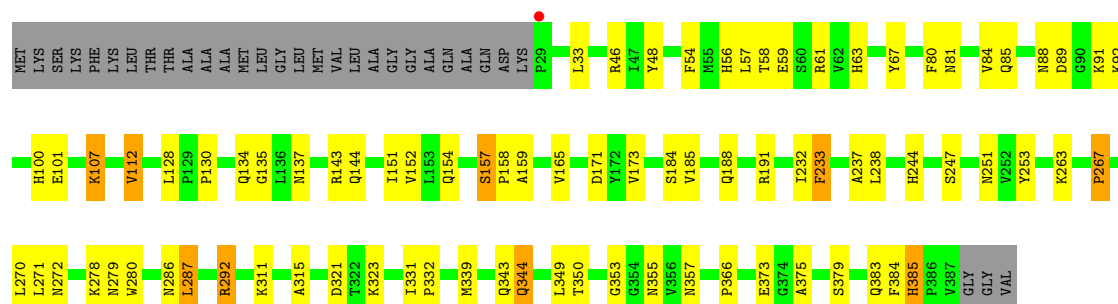
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	226	Total 226	O 226	0	0
5	B	76	Total 76	O 76	0	0
5	C	32	Total 32	O 32	0	0
5	D	228	Total 228	O 228	0	0
5	E	63	Total 63	O 63	0	0
5	F	26	Total 26	O 26	0	0

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.

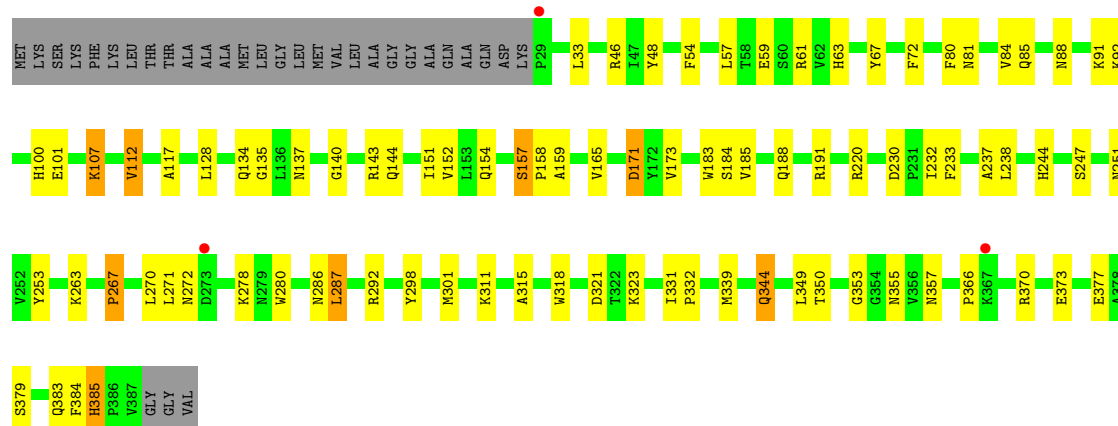
• Molecule 1: Aromatic Amine Dehydrogenase

Chain A: 



• Molecule 1: Aromatic Amine Dehydrogenase

Chain D: 



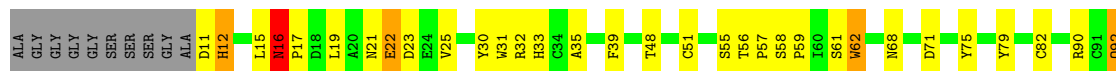
• Molecule 2: Aromatic Amine Dehydrogenase

Chain B: 

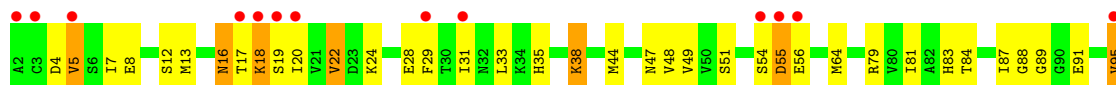




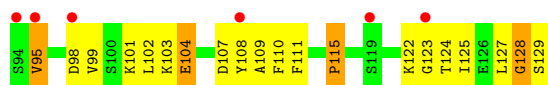
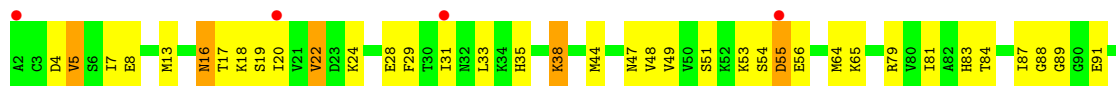
• Molecule 2: Aromatic Amine Dehydrogenase



• Molecule 3: Azurin



• Molecule 3: Azurin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.95Å 94.76Å 211.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50 40.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	71.5 (40.00-2.50) 71.8 (40.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.230 0.184 , 0.229	Depositor DCC
R_{free} test set	3401 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.9	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	0.94	EDS
Total number of atoms	10086	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: TRQ, CU

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	0.36	0/2870	0.94	15/3890 (0.4%)
1	D	0.36	0/2870	0.95	17/3890 (0.4%)
2	B	0.41	0/964	1.04	10/1313 (0.8%)
2	E	0.40	0/959	1.07	9/1306 (0.7%)
3	C	0.35	0/973	0.90	1/1307 (0.1%)
3	F	0.34	0/973	0.90	1/1307 (0.1%)
All	All	0.37	0/9609	0.96	53/13013 (0.4%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	16	ASN	CA-C-N	7.50	127.37	119.05
2	B	16	ASN	C-N-CA	7.50	127.37	119.05
1	D	137	ASN	N-CA-C	7.42	120.75	109.62
1	A	137	ASN	N-CA-C	7.17	120.78	109.39
2	E	104	GLU	N-CA-C	-7.11	99.80	109.54
1	D	385	HIS	N-CA-C	-6.89	101.38	109.93
2	E	16	ASN	CA-C-N	6.80	126.32	119.24
2	E	16	ASN	C-N-CA	6.80	126.32	119.24
1	A	287	LEU	N-CA-C	6.77	121.53	113.28
1	D	287	LEU	N-CA-C	6.76	121.36	113.18
2	B	104	GLU	N-CA-C	-6.73	100.33	109.54
2	E	120	SER	N-CA-C	6.64	121.24	113.20
1	A	385	HIS	N-CA-C	-6.62	101.72	109.93
1	A	286	ASN	N-CA-C	-6.29	100.18	109.62
2	B	120	SER	N-CA-C	6.22	120.87	113.16
1	A	173	VAL	N-CA-C	6.21	120.86	113.22
1	A	270	LEU	N-CA-C	-6.20	105.68	113.18
1	A	238	LEU	N-CA-C	6.19	119.24	109.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	238	LEU	N-CA-C	6.18	119.22	109.96
1	A	233	PHE	N-CA-C	-6.15	101.38	110.48
1	D	233	PHE	N-CA-C	-6.06	101.51	110.48
1	D	271	LEU	N-CA-C	6.04	119.67	109.76
1	D	173	VAL	N-CA-C	6.04	120.65	113.22
1	A	271	LEU	N-CA-C	6.00	119.60	109.76
1	D	270	LEU	N-CA-C	-5.87	106.08	113.18
1	D	286	ASN	N-CA-C	-5.84	100.10	109.39
1	D	117	ALA	N-CA-C	5.77	117.57	111.28
2	E	82	CYS	N-CA-C	-5.76	99.80	109.07
1	D	46	ARG	N-CA-C	5.69	119.18	110.20
3	C	55	ASP	N-CA-C	-5.68	104.56	113.02
3	F	55	ASP	N-CA-C	-5.65	104.60	113.02
1	A	272	ASN	N-CA-C	-5.58	101.49	110.14
2	E	105	PHE	N-CA-C	5.55	120.53	111.37
1	D	272	ASN	N-CA-C	-5.55	101.82	110.42
2	B	107	LEU	N-CA-C	-5.52	105.33	113.61
2	B	105	PHE	N-CA-C	5.51	120.46	111.37
2	E	31	TRP	N-CA-C	5.51	118.00	111.33
1	D	315	ALA	N-CA-C	-5.46	104.97	111.69
2	B	31	TRP	N-CA-C	5.40	117.86	111.33
2	B	82	CYS	N-CA-C	-5.32	100.50	109.07
2	E	115	MET	N-CA-C	5.31	118.54	111.75
1	A	315	ALA	N-CA-C	-5.29	105.18	111.69
1	A	46	ARG	N-CA-C	5.25	118.79	109.96
1	D	292	ARG	N-CA-C	5.23	117.38	111.11
1	D	159	ALA	N-CA-C	-5.22	102.66	110.23
2	B	114	CYS	N-CA-C	-5.21	106.60	113.17
2	B	115	MET	N-CA-C	5.20	118.41	111.75
1	D	112	VAL	N-CA-C	-5.19	100.85	108.11
1	A	159	ALA	N-CA-C	-5.18	102.72	110.23
2	E	107	LEU	N-CA-C	-5.11	105.94	113.61
1	D	140	GLY	N-CA-C	5.11	120.07	114.40
1	A	112	VAL	N-CA-C	-5.11	100.96	108.11
1	A	292	ARG	N-CA-C	5.04	117.15	111.11

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	2805	0	2749	61	0
1	D	2805	0	2749	69	0
2	B	956	0	842	45	0
2	E	951	0	837	57	0
3	C	958	0	932	58	0
3	F	958	0	932	59	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
5	A	226	0	0	2	0
5	B	76	0	0	0	0
5	C	32	0	0	2	0
5	D	228	0	0	2	0
5	E	63	0	0	0	0
5	F	26	0	0	1	0
All	All	10086	0	9041	316	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 17.

All (316) 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:21:ASN:HD21	2:B:23:ASP:HB2	1.14	1.06
2:B:92:GLN:HE21	2:B:93:CYS:N	1.55	1.03
2:E:92:GLN:HE21	2:E:93:CYS:N	1.55	1.02
2:B:62:TRQ:HB2	2:B:113:TRP:NE1	1.74	1.00
2:E:62:TRQ:HB2	2:E:113:TRP:NE1	1.76	1.00
2:E:16:ASN:HD21	2:E:19:LEU:HG	1.29	0.94
2:B:62:TRQ:HB2	2:B:113:TRP:HE1	1.33	0.89
2:E:62:TRQ:HB2	2:E:113:TRP:HE1	1.35	0.89
2:E:21:ASN:HD21	2:E:23:ASP:HB2	1.37	0.87
1:A:112:VAL:HG23	1:A:128:LEU:HD11	1.60	0.83
2:E:92:GLN:NE2	2:E:93:CYS:N	2.27	0.82
1:D:112:VAL:HG23	1:D:128:LEU:HD11	1.61	0.82
2:B:92:GLN:NE2	2:B:93:CYS:N	2.27	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:ASN:OD1	2:B:121:THR:HG23	1.79	0.82
2:E:119:ASN:OD1	2:E:121:THR:HG23	1.79	0.81
2:B:106:PHE:CE2	3:C:13:MET:HE1	2.15	0.81
2:B:21:ASN:ND2	2:B:23:ASP:HB2	1.96	0.81
2:B:92:GLN:HE21	2:B:92:GLN:C	1.89	0.80
1:D:54:PHE:CZ	2:E:92:GLN:HG3	2.16	0.80
2:E:92:GLN:HE21	2:E:92:GLN:C	1.90	0.80
2:E:16:ASN:ND2	2:E:19:LEU:HG	1.99	0.78
1:D:54:PHE:HZ	2:E:92:GLN:HG3	1.48	0.77
3:F:33:LEU:HG	3:F:87:ILE:HD11	1.67	0.76
2:B:11:ASP:O	2:B:12:HIS:HB2	1.88	0.73
3:C:33:LEU:HG	3:C:87:ILE:HD11	1.69	0.73
1:A:81:ASN:HD21	1:A:135:GLY:H	1.33	0.72
3:C:8:GLU:H	3:C:16:ASN:ND2	1.88	0.72
2:E:106:PHE:CZ	3:F:13:MET:HE1	2.25	0.72
2:B:16:ASN:OD1	2:B:19:LEU:HD12	1.90	0.72
3:F:8:GLU:H	3:F:16:ASN:ND2	1.89	0.71
1:D:81:ASN:HD21	1:D:135:GLY:H	1.36	0.71
3:F:5:VAL:HG12	3:F:31:ILE:HG13	1.74	0.70
3:C:5:VAL:HG12	3:C:31:ILE:HG13	1.74	0.70
3:F:55:ASP:OD2	3:F:79:ARG:HD2	1.92	0.70
1:A:88:ASN:H	1:A:144:GLN:HE22	1.41	0.69
3:C:55:ASP:OD2	3:C:79:ARG:HD2	1.91	0.69
1:D:88:ASN:H	1:D:144:GLN:HE22	1.39	0.69
2:E:92:GLN:HE21	2:E:93:CYS:H	1.40	0.69
2:B:90:ARG:HG3	2:B:90:ARG:HH11	1.58	0.68
3:F:28:GLU:HA	3:F:98:ASP:HA	1.75	0.68
3:F:103:LYS:HB2	3:F:108:TYR:OH	1.93	0.68
2:E:21:ASN:ND2	2:E:23:ASP:HB2	2.09	0.68
2:E:90:ARG:HG3	2:E:90:ARG:HH11	1.57	0.68
3:C:28:GLU:HA	3:C:98:ASP:HA	1.74	0.68
3:C:103:LYS:HB2	3:C:108:TYR:OH	1.93	0.67
1:A:188:GLN:NE2	1:A:191:ARG:HH11	1.93	0.66
3:F:127:LEU:HD12	3:F:128:GLY:H	1.60	0.66
3:C:38:LYS:HG3	3:C:38:LYS:O	1.96	0.66
3:C:127:LEU:HD12	3:C:128:GLY:H	1.60	0.66
1:A:54:PHE:CZ	2:B:92:GLN:HG3	2.31	0.65
1:D:188:GLN:NE2	1:D:191:ARG:HH11	1.95	0.65
1:A:61:ARG:HH11	1:A:63:HIS:HE1	1.46	0.64
1:A:154:GLN:HE21	1:A:184:SER:H	1.45	0.64
1:A:54:PHE:HZ	2:B:92:GLN:HG3	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:ARG:HH11	1:D:63:HIS:HE1	1.46	0.63
1:D:143:ARG:HH22	1:D:383:GLN:NE2	1.96	0.63
3:F:38:LYS:O	3:F:38:LYS:HG3	1.96	0.63
2:B:92:GLN:HE21	2:B:93:CYS:H	1.42	0.63
2:E:39:PHE:CE2	2:E:92:GLN:HG2	2.34	0.63
1:D:311:LYS:HZ2	2:E:96:GLN:NE2	1.96	0.63
1:D:251:ASN:HB3	1:D:267:PRO:HB2	1.81	0.62
1:D:232:ILE:HA	1:D:247:SER:HA	1.82	0.62
2:B:59:PRO:O	3:C:12:SER:HA	2.00	0.62
1:D:154:GLN:HE21	1:D:184:SER:H	1.47	0.62
3:C:84:THR:HG22	3:C:95:VAL:HB	1.82	0.62
1:D:154:GLN:NE2	1:D:184:SER:H	1.98	0.62
1:A:143:ARG:HH22	1:A:383:GLN:NE2	1.98	0.61
2:B:39:PHE:CE2	2:B:92:GLN:HG2	2.35	0.61
3:F:84:THR:HG22	3:F:95:VAL:HB	1.82	0.61
1:A:154:GLN:NE2	1:A:184:SER:H	1.99	0.61
3:C:33:LEU:HD22	3:C:48:VAL:HG23	1.83	0.61
3:F:33:LEU:HD22	3:F:48:VAL:HG23	1.83	0.60
1:A:232:ILE:HA	1:A:247:SER:HA	1.82	0.60
1:A:134:GLN:HE22	2:B:120:SER:HB2	1.67	0.60
3:C:17:THR:HG22	3:C:19:SER:H	1.67	0.59
3:F:17:THR:HG22	3:F:19:SER:H	1.67	0.59
3:C:5:VAL:HG11	3:C:20:ILE:HD13	1.84	0.59
1:A:251:ASN:HB3	1:A:267:PRO:HB2	1.82	0.59
2:E:92:GLN:HE21	2:E:92:GLN:CA	2.15	0.59
3:F:44:MET:O	3:F:44:MET:HG3	2.02	0.59
2:B:92:GLN:HE21	2:B:92:GLN:CA	2.15	0.58
3:F:53:LYS:HG3	5:F:343:HOH:O	2.03	0.58
2:B:30:TYR:HB3	2:B:33:HIS:CD2	2.38	0.58
3:F:51:SER:HA	3:F:81:ILE:HD13	1.85	0.58
3:F:5:VAL:HG11	3:F:20:ILE:HD13	1.85	0.58
3:C:44:MET:O	3:C:44:MET:HG3	2.04	0.57
3:F:102:LEU:HD22	3:F:108:TYR:CD2	2.39	0.57
1:D:311:LYS:NZ	2:E:96:GLN:NE2	2.52	0.57
2:E:30:TYR:HB3	2:E:33:HIS:CD2	2.40	0.57
2:B:106:PHE:CZ	3:C:13:MET:HE1	2.39	0.57
3:C:102:LEU:HD22	3:C:108:TYR:CD2	2.39	0.57
1:D:88:ASN:H	1:D:144:GLN:NE2	2.03	0.56
3:F:104:GLU:OE1	3:F:104:GLU:N	2.38	0.56
3:C:104:GLU:OE1	3:C:104:GLU:N	2.38	0.56
3:C:51:SER:HA	3:C:81:ILE:HD13	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:11:ASP:O	2:E:12:HIS:HB2	2.04	0.56
3:F:110:PHE:CZ	3:F:123:GLY:HA3	2.41	0.55
2:E:58:SER:HA	2:E:117:ASN:HD21	1.72	0.55
1:A:237:ALA:HB3	1:A:244:HIS:HB2	1.88	0.55
2:E:62:TRQ:CB	2:E:113:TRP:NE1	2.63	0.55
2:B:108:HIS:CE1	2:B:110:ASP:HB2	2.42	0.55
1:A:84:VAL:HG22	1:A:85:GLN:N	2.21	0.55
2:E:108:HIS:CE1	2:E:110:ASP:HB2	2.41	0.55
1:D:48:TYR:OH	1:D:385:HIS:HD2	1.90	0.55
1:A:56:HIS:NE2	1:D:377:GLU:OE2	2.33	0.54
2:B:58:SER:HA	2:B:117:ASN:HD21	1.72	0.54
2:E:15:LEU:HD21	2:E:75:TYR:CZ	2.42	0.54
1:D:84:VAL:HG22	1:D:85:GLN:N	2.22	0.54
2:B:35:ALA:HB3	2:B:79:TYR:CE1	2.41	0.54
2:E:35:ALA:HB3	2:E:79:TYR:CE1	2.43	0.54
1:D:237:ALA:HB3	1:D:244:HIS:HB2	1.88	0.54
3:C:110:PHE:CZ	3:C:123:GLY:HA3	2.42	0.54
1:D:143:ARG:HH22	1:D:383:GLN:HE22	1.56	0.54
3:F:128:GLY:O	3:F:129:SER:HB2	2.07	0.54
1:D:134:GLN:HE22	2:E:120:SER:HB2	1.73	0.54
1:D:344:GLN:HB2	5:D:527:HOH:O	2.07	0.54
3:F:5:VAL:HG21	3:F:20:ILE:HG23	1.90	0.54
3:C:5:VAL:HG21	3:C:20:ILE:HG23	1.89	0.53
3:C:128:GLY:O	3:C:129:SER:HB2	2.07	0.53
3:C:22:VAL:HG12	3:C:29:PHE:CE1	2.43	0.53
3:C:99:VAL:C	3:C:101:LYS:H	2.16	0.53
3:C:127:LEU:HD12	3:C:128:GLY:N	2.23	0.53
3:F:22:VAL:HG12	3:F:29:PHE:CE1	2.43	0.53
1:A:61:ARG:HH11	1:A:63:HIS:CE1	2.27	0.53
3:C:24:LYS:HG3	3:C:128:GLY:HA3	1.90	0.53
1:D:339:MET:HA	1:D:349:LEU:O	2.09	0.53
2:B:62:TRQ:CB	2:B:113:TRP:NE1	2.61	0.53
3:F:24:LYS:HG3	3:F:128:GLY:HA3	1.91	0.53
3:F:31:ILE:HG23	3:F:31:ILE:O	2.09	0.53
1:D:134:GLN:NE2	2:E:112:ASN:HD22	2.07	0.52
2:E:106:PHE:CE2	3:F:13:MET:HE1	2.44	0.52
3:F:127:LEU:HD12	3:F:128:GLY:N	2.23	0.52
2:E:16:ASN:OD1	2:E:19:LEU:HD12	2.09	0.52
1:A:339:MET:HA	1:A:349:LEU:O	2.10	0.52
2:E:22:GLU:HA	2:E:25:VAL:HG22	1.90	0.52
2:E:90:ARG:HG3	2:E:90:ARG:NH1	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:92:GLN:NE2	2:E:93:CYS:H	2.03	0.52
2:B:90:ARG:HG3	2:B:90:ARG:NH1	2.24	0.52
3:C:31:ILE:HG23	3:C:31:ILE:O	2.09	0.52
3:F:99:VAL:C	3:F:101:LYS:H	2.18	0.51
3:F:122:LYS:C	3:F:122:LYS:HD3	2.36	0.51
1:A:88:ASN:H	1:A:144:GLN:NE2	2.05	0.51
1:A:355:ASN:OD1	1:A:373:GLU:HA	2.10	0.51
3:C:122:LYS:HD3	3:C:122:LYS:C	2.35	0.51
3:F:104:GLU:CD	3:F:104:GLU:H	2.08	0.51
1:A:33:LEU:CD2	2:E:57:PRO:HB3	2.41	0.51
1:A:81:ASN:HD21	1:A:135:GLY:N	2.05	0.51
3:C:5:VAL:CG1	3:C:31:ILE:HG13	2.40	0.51
3:C:8:GLU:H	3:C:16:ASN:HD21	1.56	0.51
1:A:278:LYS:HG2	5:A:545:HOH:O	2.10	0.51
1:A:48:TYR:OH	1:A:385:HIS:HD2	1.94	0.51
1:A:353:GLY:HA2	1:A:379:SER:O	2.11	0.51
3:C:24:LYS:HG2	3:C:127:LEU:HD11	1.93	0.51
3:C:47:ASN:C	3:C:47:ASN:OD1	2.54	0.51
1:A:152:VAL:HG12	1:A:185:VAL:HG21	1.93	0.51
1:D:355:ASN:OD1	1:D:373:GLU:HA	2.10	0.51
3:F:47:ASN:OD1	3:F:47:ASN:C	2.54	0.50
1:A:350:THR:OG1	1:A:357:ASN:HB2	2.11	0.50
3:F:24:LYS:HG2	3:F:127:LEU:HD11	1.94	0.50
1:A:331:ILE:HD13	1:A:366:PRO:HB2	1.94	0.50
1:D:350:THR:OG1	1:D:357:ASN:HB2	2.12	0.50
1:A:57:LEU:O	1:A:80:PHE:HA	2.12	0.50
3:C:104:GLU:CD	3:C:104:GLU:H	2.08	0.50
3:C:7:ILE:HG23	3:C:33:LEU:HD13	1.92	0.49
3:F:5:VAL:CG1	3:F:31:ILE:HG13	2.39	0.49
1:D:321:ASP:OD1	1:D:323:LYS:HB2	2.13	0.49
3:F:49:VAL:HG22	3:F:83:HIS:HB2	1.94	0.49
1:A:143:ARG:HH22	1:A:383:GLN:HE22	1.60	0.49
1:D:61:ARG:HH11	1:D:63:HIS:CE1	2.27	0.49
1:D:91:LYS:O	1:D:92:LYS:HD3	2.12	0.49
1:D:220:ARG:HH21	3:F:64:MET:CE	2.25	0.49
1:D:157:SER:N	1:D:158:PRO:HA	2.27	0.49
1:A:157:SER:N	1:A:158:PRO:HA	2.27	0.49
2:B:51:CYS:HB3	2:B:55:SER:OG	2.13	0.49
2:E:51:CYS:HB3	2:E:55:SER:OG	2.13	0.49
3:C:16:ASN:N	3:C:16:ASN:HD22	2.11	0.48
3:F:109:ALA:HB1	3:F:123:GLY:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:GLN:NE2	2:B:112:ASN:HD22	2.11	0.48
2:B:57:PRO:HB3	1:D:33:LEU:CD2	2.44	0.48
1:D:152:VAL:HG12	1:D:185:VAL:HG21	1.94	0.48
3:F:7:ILE:HG23	3:F:33:LEU:HD13	1.94	0.48
3:C:49:VAL:HG22	3:C:83:HIS:HB2	1.96	0.48
3:C:109:ALA:HB1	3:C:123:GLY:O	2.14	0.48
1:D:331:ILE:HD13	1:D:366:PRO:HB2	1.96	0.48
1:A:311:LYS:HZ2	2:B:96:GLN:NE2	2.12	0.48
1:A:33:LEU:HD23	2:E:57:PRO:HB3	1.95	0.48
1:A:233:PHE:HB3	5:A:451:HOH:O	2.14	0.48
1:D:57:LEU:O	1:D:80:PHE:HA	2.14	0.47
3:F:16:ASN:N	3:F:16:ASN:HD22	2.12	0.47
3:C:7:ILE:O	3:C:33:LEU:HD12	2.13	0.47
1:A:253:TYR:CZ	1:A:267:PRO:HB3	2.50	0.47
1:D:353:GLY:HA2	1:D:379:SER:O	2.14	0.47
2:E:62:TRQ:HB2	2:E:113:TRP:CE2	2.49	0.47
1:A:349:LEU:HG	1:A:384:PHE:CE1	2.50	0.47
1:D:349:LEU:HG	1:D:384:PHE:CE1	2.50	0.47
3:F:7:ILE:O	3:F:33:LEU:HD12	2.14	0.47
1:A:321:ASP:OD1	1:A:323:LYS:HB2	2.15	0.46
2:E:134:LYS:HE3	2:E:134:LYS:HB3	1.74	0.46
1:D:54:PHE:CE1	2:E:92:GLN:CG	2.98	0.46
1:A:100:HIS:HA	1:A:107:LYS:O	2.15	0.46
2:B:86:THR:HG21	1:D:59:GLU:HG3	1.97	0.46
1:D:81:ASN:HD21	1:D:135:GLY:N	2.08	0.46
1:A:91:LYS:O	1:A:92:LYS:HD3	2.15	0.46
2:B:32:ARG:HD2	2:B:48:THR:HG21	1.96	0.46
1:D:220:ARG:NH2	3:F:64:MET:CE	2.78	0.46
2:E:32:ARG:HD2	2:E:48:THR:HG21	1.98	0.46
2:B:16:ASN:OD1	2:B:19:LEU:HB2	2.16	0.46
3:F:13:MET:HE3	3:F:13:MET:HB2	1.70	0.46
1:D:253:TYR:CZ	1:D:267:PRO:HB3	2.51	0.46
3:C:18:LYS:HE2	5:C:145:HOH:O	2.15	0.45
1:A:349:LEU:HG	1:A:384:PHE:CZ	2.51	0.45
1:A:344:GLN:HE21	1:A:344:GLN:HB3	1.58	0.45
3:C:5:VAL:HG21	3:C:20:ILE:CG2	2.47	0.45
3:C:64:MET:HB2	5:C:143:HOH:O	2.15	0.45
3:C:99:VAL:C	3:C:101:LYS:N	2.74	0.45
1:D:349:LEU:HG	1:D:384:PHE:CZ	2.51	0.45
2:E:17:PRO:HD3	2:E:32:ARG:NH2	2.31	0.45
3:C:102:LEU:HD22	3:C:108:TYR:CG	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLU:O	1:A:59:GLU:HG2	2.17	0.45
3:F:35:HIS:ND1	3:F:89:GLY:HA2	2.32	0.45
3:F:8:GLU:H	3:F:16:ASN:HD21	1.59	0.45
3:C:87:ILE:HB	3:C:91:GLU:HB2	1.99	0.45
1:D:100:HIS:HA	1:D:107:LYS:O	2.16	0.45
1:A:157:SER:N	1:A:158:PRO:CA	2.80	0.44
1:D:220:ARG:NH2	3:F:64:MET:HE3	2.32	0.44
1:D:311:LYS:HD2	2:E:96:GLN:CD	2.43	0.44
3:F:81:ILE:HD12	3:F:81:ILE:N	2.32	0.44
3:F:102:LEU:HD22	3:F:108:TYR:CG	2.52	0.44
3:F:125:ILE:HG23	3:F:125:ILE:O	2.17	0.44
2:B:62:TRQ:HB2	2:B:113:TRP:CE2	2.48	0.44
3:C:81:ILE:HD12	3:C:81:ILE:N	2.32	0.44
3:F:22:VAL:HG22	3:F:127:LEU:HA	1.99	0.44
3:F:87:ILE:HB	3:F:91:GLU:HB2	2.00	0.44
2:B:92:GLN:NE2	2:B:93:CYS:H	2.05	0.44
2:E:108:HIS:NE2	2:E:110:ASP:HB2	2.33	0.44
1:D:183:TRP:CD1	2:E:102:GLY:HA3	2.53	0.44
1:A:151:ILE:HB	1:A:165:VAL:HB	2.00	0.44
2:E:59:PRO:HD2	2:E:117:ASN:HD21	1.83	0.44
3:C:56:GLU:HG3	3:C:111:PHE:CE1	2.52	0.44
1:D:157:SER:N	1:D:158:PRO:CA	2.81	0.44
2:B:108:HIS:NE2	2:B:110:ASP:HB2	2.33	0.43
3:F:5:VAL:HG21	3:F:20:ILE:CG2	2.48	0.43
2:B:16:ASN:HD21	2:B:19:LEU:HG	1.82	0.43
2:B:59:PRO:HD2	2:B:117:ASN:HD21	1.83	0.43
3:C:35:HIS:ND1	3:C:89:GLY:HA2	2.32	0.43
1:A:63:HIS:HD2	1:A:375:ALA:O	2.02	0.43
3:F:56:GLU:HG3	3:F:111:PHE:CE1	2.52	0.43
1:A:84:VAL:CG2	1:A:85:GLN:N	2.82	0.43
1:D:61:ARG:NH1	1:D:63:HIS:HE1	2.15	0.43
1:D:151:ILE:HB	1:D:165:VAL:HB	2.01	0.43
2:B:61:SER:HB2	2:B:79:TYR:C	2.44	0.43
1:D:370:ARG:HD3	5:D:392:HOH:O	2.18	0.43
3:C:22:VAL:HG22	3:C:127:LEU:HA	2.00	0.43
3:C:122:LYS:HD3	3:C:123:GLY:N	2.34	0.43
3:C:125:ILE:O	3:C:125:ILE:HG23	2.17	0.43
2:E:11:ASP:O	2:E:12:HIS:CB	2.66	0.43
2:E:17:PRO:C	2:E:19:LEU:N	2.76	0.43
3:F:22:VAL:O	3:F:22:VAL:CG2	2.67	0.43
1:A:101:GLU:CD	1:A:107:LYS:HB2	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:GLN:NE2	2:B:92:GLN:C	2.69	0.42
1:D:230:ASP:OD2	1:D:253:TYR:OH	2.33	0.42
1:D:101:GLU:CD	1:D:107:LYS:HB2	2.44	0.42
1:D:154:GLN:HE21	1:D:184:SER:N	2.16	0.42
3:C:19:SER:HA	3:C:124:THR:O	2.18	0.42
2:B:44:CYS:HA	1:D:72:PHE:CD2	2.54	0.42
1:D:67:TYR:CD1	1:D:67:TYR:C	2.97	0.42
1:A:61:ARG:HD2	1:A:61:ARG:N	2.35	0.42
1:A:188:GLN:HE22	1:A:191:ARG:HH11	1.66	0.42
1:D:54:PHE:CE1	2:E:92:GLN:HG3	2.53	0.42
2:E:92:GLN:NE2	2:E:92:GLN:C	2.70	0.42
3:C:109:ALA:HB1	3:C:122:LYS:HE2	2.02	0.42
1:D:59:GLU:O	1:D:59:GLU:HG2	2.18	0.42
1:D:61:ARG:N	1:D:61:ARG:HD2	2.34	0.42
3:F:99:VAL:C	3:F:101:LYS:N	2.75	0.42
3:C:83:HIS:C	3:C:95:VAL:HG21	2.45	0.42
3:F:19:SER:HA	3:F:124:THR:O	2.20	0.42
2:E:16:ASN:CG	2:E:19:LEU:HG	2.43	0.42
3:F:35:HIS:HB3	3:F:88:GLY:O	2.19	0.42
1:A:278:LYS:HB2	1:A:280:TRP:CD1	2.54	0.42
2:E:16:ASN:CG	2:E:16:ASN:O	2.63	0.42
2:E:61:SER:HB2	2:E:79:TYR:C	2.45	0.41
2:E:16:ASN:HA	2:E:17:PRO:HD3	1.82	0.41
2:E:56:THR:HA	2:E:57:PRO:HD3	1.93	0.41
3:C:35:HIS:HB3	3:C:88:GLY:O	2.19	0.41
3:F:109:ALA:HA	3:F:124:THR:HA	2.02	0.41
1:A:61:ARG:NH1	1:A:63:HIS:HE1	2.15	0.41
3:C:102:LEU:HD23	3:C:102:LEU:HA	1.92	0.41
3:F:109:ALA:HB1	3:F:122:LYS:HE2	2.01	0.41
1:A:311:LYS:NZ	2:B:96:GLN:NE2	2.69	0.41
1:A:292:ARG:H	1:A:343:GLN:HE22	1.69	0.41
3:C:8:GLU:HB2	3:C:16:ASN:CG	2.46	0.41
1:D:54:PHE:CZ	2:E:92:GLN:CG	2.97	0.41
1:D:278:LYS:HB2	1:D:280:TRP:CD1	2.55	0.41
2:E:68:ASN:HB3	2:E:71:ASP:OD1	2.20	0.41
3:F:122:LYS:HD3	3:F:123:GLY:N	2.35	0.41
2:B:16:ASN:HA	2:B:17:PRO:HD3	1.75	0.41
1:A:89:ASP:C	1:A:89:ASP:OD1	2.64	0.41
1:A:278:LYS:O	1:A:279:ASN:HB2	2.21	0.41
2:B:99:GLU:OE2	2:B:108:HIS:HD2	2.04	0.41
2:E:16:ASN:OD1	2:E:19:LEU:CD1	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLN:NE2	1:A:191:ARG:HD2	2.36	0.41
1:D:220:ARG:CD	3:F:65:LYS:HD3	2.51	0.41
1:D:331:ILE:HB	1:D:332:PRO:CD	2.51	0.41
1:A:67:TYR:CD1	1:A:67:TYR:C	2.98	0.40
1:A:188:GLN:NE2	1:A:191:ARG:NH1	2.65	0.40
3:C:22:VAL:O	3:C:22:VAL:CG2	2.67	0.40
3:C:98:ASP:OD1	3:C:98:ASP:N	2.48	0.40
1:D:165:VAL:HA	1:D:171:ASP:O	2.21	0.40
3:F:83:HIS:C	3:F:95:VAL:HG21	2.46	0.40
1:D:298:TYR:CD1	1:D:298:TYR:N	2.89	0.40
1:A:58:THR:OG1	1:D:59:GLU:OE1	2.29	0.40
1:D:84:VAL:CG2	1:D:85:GLN:N	2.84	0.40
1:A:331:ILE:HB	1:A:332:PRO:CD	2.52	0.40
1:D:301:MET:HE2	1:D:318:TRP:CE3	2.57	0.40
2:B:68:ASN:HB3	2:B:71:ASP:OD1	2.21	0.40
1:D:188:GLN:NE2	1:D:191:ARG:HD2	2.37	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	357/390 (92%)	331 (93%)	24 (7%)	2 (1%)	21	38
1	D	357/390 (92%)	334 (94%)	22 (6%)	1 (0%)	36	55
2	B	122/135 (90%)	112 (92%)	8 (7%)	2 (2%)	7	14
2	E	121/135 (90%)	113 (93%)	7 (6%)	1 (1%)	16	31
3	C	126/128 (98%)	112 (89%)	12 (10%)	2 (2%)	7	14
3	F	126/128 (98%)	112 (89%)	12 (10%)	2 (2%)	7	14
All	All	1209/1306 (93%)	1114 (92%)	85 (7%)	10 (1%)	16	31

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	11	ASP
2	B	12	HIS
2	E	12	HIS
3	C	128	GLY
3	F	128	GLY
3	C	115	PRO
3	F	115	PRO
1	D	157	SER
1	A	157	SER
1	A	130	PRO

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	305/325 (94%)	299 (98%)	6 (2%)	48 75
1	D	305/325 (94%)	299 (98%)	6 (2%)	48 75
2	B	108/112 (96%)	101 (94%)	7 (6%)	15 32
2	E	108/112 (96%)	102 (94%)	6 (6%)	19 39
3	C	106/106 (100%)	95 (90%)	11 (10%)	7 14
3	F	106/106 (100%)	95 (90%)	11 (10%)	7 14
All	All	1038/1086 (96%)	991 (96%)	47 (4%)	24 49

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	LYS
1	A	171	ASP
1	A	263	LYS
1	A	267	PRO
1	A	287	LEU
1	A	344	GLN
2	B	13	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	16	ASN
2	B	21	ASN
2	B	92	GLN
2	B	98	ARG
2	B	121	THR
2	B	134	LYS
3	C	4	ASP
3	C	5	VAL
3	C	16	ASN
3	C	18	LYS
3	C	22	VAL
3	C	38	LYS
3	C	54	SER
3	C	95	VAL
3	C	104	GLU
3	C	107	ASP
3	C	115	PRO
1	D	107	LYS
1	D	171	ASP
1	D	263	LYS
1	D	267	PRO
1	D	287	LEU
1	D	344	GLN
2	E	16	ASN
2	E	22	GLU
2	E	92	GLN
2	E	98	ARG
2	E	121	THR
2	E	134	LYS
3	F	4	ASP
3	F	5	VAL
3	F	16	ASN
3	F	18	LYS
3	F	22	VAL
3	F	38	LYS
3	F	54	SER
3	F	95	VAL
3	F	104	GLU
3	F	107	ASP
3	F	115	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	63	HIS
1	A	81	ASN
1	A	85	GLN
1	A	100	HIS
1	A	134	GLN
1	A	137	ASN
1	A	144	GLN
1	A	154	GLN
1	A	188	GLN
1	A	223	GLN
1	A	343	GLN
1	A	344	GLN
1	A	383	GLN
1	A	385	HIS
2	B	21	ASN
2	B	92	GLN
2	B	96	GLN
2	B	108	HIS
2	B	117	ASN
3	C	14	GLN
3	C	16	ASN
3	C	32	ASN
1	D	43	GLN
1	D	63	HIS
1	D	81	ASN
1	D	85	GLN
1	D	100	HIS
1	D	134	GLN
1	D	137	ASN
1	D	144	GLN
1	D	154	GLN
1	D	188	GLN
1	D	208	ASN
1	D	223	GLN
1	D	343	GLN
1	D	344	GLN
1	D	346	ASN
1	D	381	GLN
1	D	383	GLN
1	D	385	HIS
2	E	21	ASN
2	E	92	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	94	ASN
2	E	96	GLN
2	E	108	HIS
2	E	117	ASN
3	F	16	ASN
3	F	32	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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$
2	TRQ	E	62	2	16,17,18	1.50	3 (18%)	16,24,26	1.61	2 (12%)
2	TRQ	B	62	2	16,17,18	1.48	3 (18%)	16,24,26	1.94	3 (18%)

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
2	TRQ	E	62	2	-	0/5/19/21	0/2/2/2
2	TRQ	B	62	2	-	0/5/19/21	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	62	TRQ	CH2-CZ2	-3.45	1.37	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	62	TRQ	CH2-CZ2	-3.38	1.37	1.53
2	E	62	TRQ	CE2-CZ2	-2.74	1.40	1.50
2	B	62	TRQ	CE2-CZ2	-2.70	1.40	1.50
2	E	62	TRQ	CD2-CG	2.10	1.46	1.42
2	B	62	TRQ	CE3-CZ3	2.06	1.40	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	62	TRQ	O7-CZ2-CH2	5.78	125.76	118.39
2	E	62	TRQ	O7-CZ2-CH2	4.56	124.20	118.39
2	B	62	TRQ	O6-CH2-CZ3	-3.00	116.18	121.58
2	E	62	TRQ	O6-CH2-CZ3	-2.44	117.20	121.58
2	B	62	TRQ	O6-CH2-CZ2	2.31	122.43	118.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	62	TRQ	4	0
2	B	62	TRQ	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	359/390 (92%)	-0.47	1 (0%) 90 87	14, 26, 44, 69	0
1	D	359/390 (92%)	-0.43	3 (0%) 82 80	13, 26, 42, 67	0
2	B	124/135 (91%)	-0.36	1 (0%) 82 80	12, 25, 54, 76	0
2	E	123/135 (91%)	-0.33	0 100 100	16, 26, 62, 76	0
3	C	128/128 (100%)	0.90	21 (16%) 4 3	31, 56, 93, 100	0
3	F	128/128 (100%)	0.78	10 (7%) 19 17	38, 61, 93, 100	0
All	All	1221/1306 (93%)	-0.16	36 (2%) 53 49	12, 28, 76, 100	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	127	LEU	3.9
1	D	29	PRO	3.5
3	C	5	VAL	3.1
3	C	20	ILE	3.1
3	C	107	ASP	3.0
1	A	29	PRO	2.9
3	F	31	ILE	2.8
3	F	2	ALA	2.7
3	C	125	ILE	2.6
3	C	126	GLU	2.6
3	C	3	CYS	2.6
3	C	19	SER	2.6
3	C	128	GLY	2.5
3	C	55	ASP	2.5
3	C	54	SER	2.4
3	C	18	LYS	2.4
3	F	94	SER	2.4
3	C	98	ASP	2.4
3	C	31	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	119	SER	2.3
3	F	108	TYR	2.3
3	C	17	THR	2.2
3	C	2	ALA	2.2
3	F	55	ASP	2.2
3	C	56	GLU	2.2
3	F	119	SER	2.1
2	B	134	LYS	2.1
3	C	29	PHE	2.1
3	F	95	VAL	2.1
1	D	273	ASP	2.1
3	F	98	ASP	2.1
3	C	95	VAL	2.1
3	F	20	ILE	2.1
1	D	367	LYS	2.1
3	C	102	LEU	2.1
3	F	123	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	TRQ	B	62	16/17	0.95	0.06	17,22,28,29	0
2	TRQ	E	62	16/17	0.97	0.07	15,23,26,28	0

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
4	CU	F	130	1/1	0.96	0.10	50,50,50,50	0
4	CU	C	130	1/1	0.98	0.11	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.