



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:29 AM UTC

PDB ID : 3E82 / pdb_00003e82
Title : Crystal structure of a putative oxidoreductase from *Klebsiella pneumoniae*
Authors : Eswaramoorthy, S.; Mohammad, M.B.; Thomas, C.A.; Brown, A.C.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2008-08-19
Resolution : 2.04 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

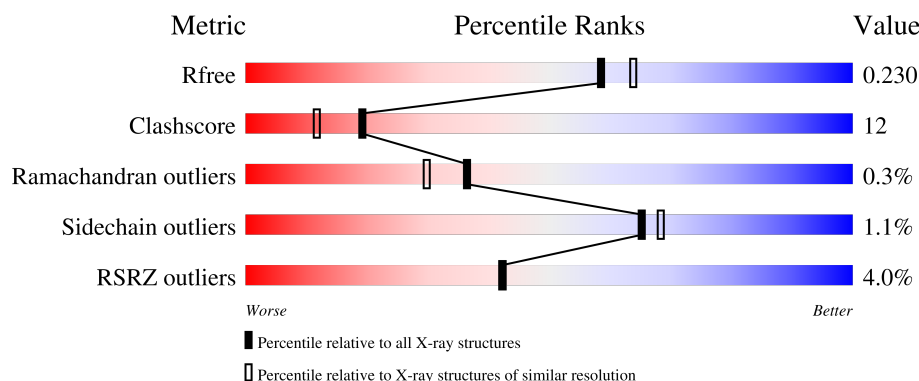
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	364	8% 72% 21% 6%
1	B	364	3% 76% 18% 5%
1	D	364	8% 73% 21% . .
1	E	364	3% 77% 16% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11358 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 Putative oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	Se	0	0	0
			2645	1669	475	495	1	5			
1	B	347	Total	C	N	O	S	Se	0	0	0
			2675	1686	481	502	1	5			
1	D	350	Total	C	N	O	S	Se	0	0	0
			2712	1710	492	504	1	5			
1	E	344	Total	C	N	O	S	Se	0	0	0
			2638	1664	472	496	1	5			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MSE	-	expression tag	UNP A6T882
A	10	SER	-	expression tag	UNP A6T882
A	11	LEU	-	expression tag	UNP A6T882
A	365	GLU	-	expression tag	UNP A6T882
A	366	GLY	-	expression tag	UNP A6T882
A	367	HIS	-	expression tag	UNP A6T882
A	368	HIS	-	expression tag	UNP A6T882
A	369	HIS	-	expression tag	UNP A6T882
A	370	HIS	-	expression tag	UNP A6T882
A	371	HIS	-	expression tag	UNP A6T882
A	372	HIS	-	expression tag	UNP A6T882
B	9	MSE	-	expression tag	UNP A6T882
B	10	SER	-	expression tag	UNP A6T882
B	11	LEU	-	expression tag	UNP A6T882
B	365	GLU	-	expression tag	UNP A6T882
B	366	GLY	-	expression tag	UNP A6T882
B	367	HIS	-	expression tag	UNP A6T882
B	368	HIS	-	expression tag	UNP A6T882
B	369	HIS	-	expression tag	UNP A6T882
B	370	HIS	-	expression tag	UNP A6T882
B	371	HIS	-	expression tag	UNP A6T882

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Chain	Residue	Modelled	Actual	Comment	Reference
B	372	HIS	-	expression tag	UNP A6T882
D	9	MSE	-	expression tag	UNP A6T882
D	10	SER	-	expression tag	UNP A6T882
D	11	LEU	-	expression tag	UNP A6T882
D	365	GLU	-	expression tag	UNP A6T882
D	366	GLY	-	expression tag	UNP A6T882
D	367	HIS	-	expression tag	UNP A6T882
D	368	HIS	-	expression tag	UNP A6T882
D	369	HIS	-	expression tag	UNP A6T882
D	370	HIS	-	expression tag	UNP A6T882
D	371	HIS	-	expression tag	UNP A6T882
D	372	HIS	-	expression tag	UNP A6T882
E	9	MSE	-	expression tag	UNP A6T882
E	10	SER	-	expression tag	UNP A6T882
E	11	LEU	-	expression tag	UNP A6T882
E	365	GLU	-	expression tag	UNP A6T882
E	366	GLY	-	expression tag	UNP A6T882
E	367	HIS	-	expression tag	UNP A6T882
E	368	HIS	-	expression tag	UNP A6T882
E	369	HIS	-	expression tag	UNP A6T882
E	370	HIS	-	expression tag	UNP A6T882
E	371	HIS	-	expression tag	UNP A6T882
E	372	HIS	-	expression tag	UNP A6T882

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	210	Total O 210 210	0	0

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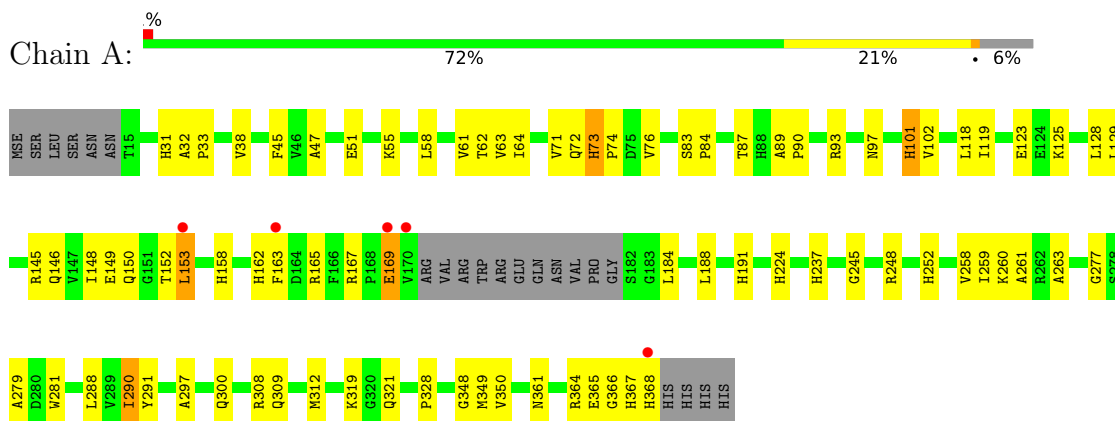
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	181	Total 181	O 181	0	0
3	D	118	Total 118	O 118	0	0
3	E	175	Total 175	O 175	0	0

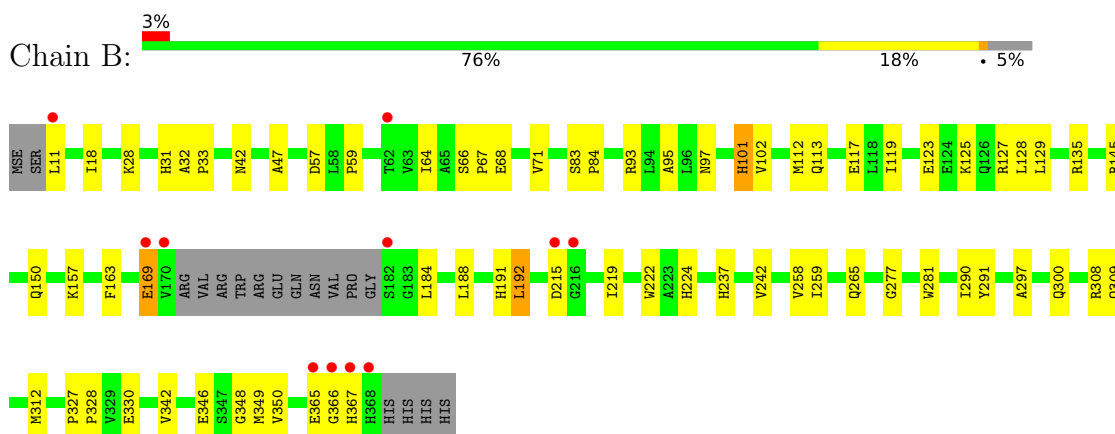
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

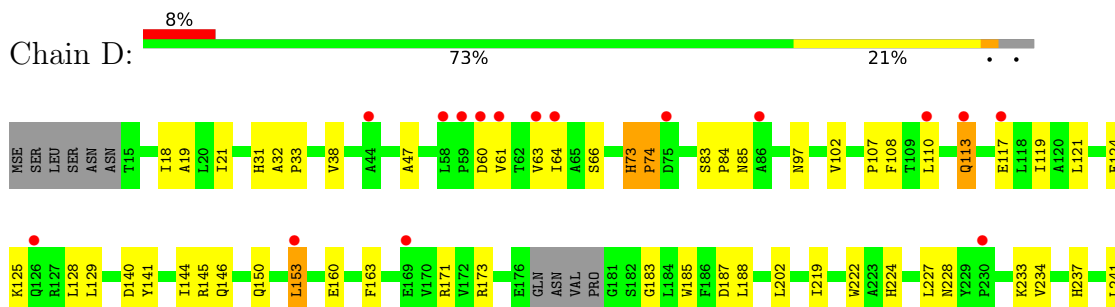
• Molecule 1: Putative oxidoreductase

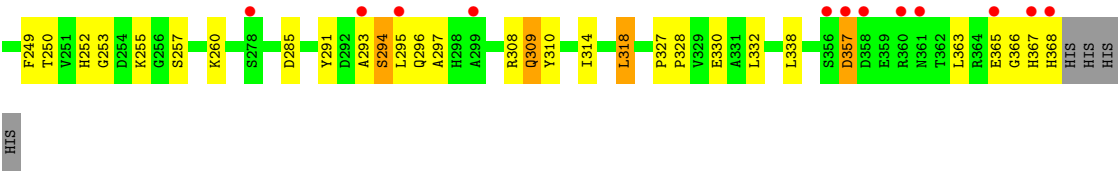


• Molecule 1: Putative oxidoreductase

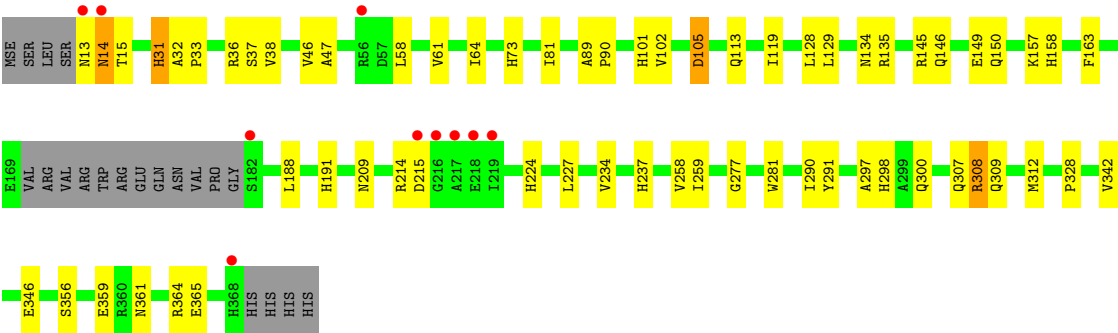
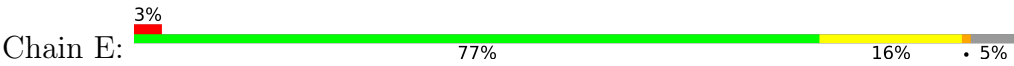


• Molecule 1: Putative oxidoreductase





● Molecule 1: Putative oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.91Å 79.75Å 209.14Å 90.00° 94.00° 90.00°	Depositor
Resolution (Å)	35.87 – 2.04 35.87 – 2.04	Depositor EDS
% Data completeness (in resolution range)	94.0 (35.87-2.04) 94.0 (35.87-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.03Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.232 0.207 , 0.230	Depositor DCC
R_{free} test set	4166 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11358	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	0.39	0/2696	0.94	10/3660 (0.3%)
1	B	0.41	0/2726	0.94	8/3701 (0.2%)
1	D	0.40	0/2765	0.92	10/3752 (0.3%)
1	E	0.41	0/2689	0.95	8/3653 (0.2%)
All	All	0.40	0/10876	0.94	36/14766 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	357	ASP	N-CA-C	8.17	120.19	111.28
1	E	15	THR	N-CA-C	-7.80	95.55	108.34
1	A	31	HIS	N-CA-C	7.76	119.37	111.07
1	E	73	HIS	CA-C-N	7.71	128.11	119.32
1	E	73	HIS	C-N-CA	7.71	128.11	119.32
1	D	102	VAL	N-CA-C	7.07	118.92	108.45
1	E	31	HIS	N-CA-C	6.94	119.49	111.02
1	A	73	HIS	CA-C-N	6.70	126.21	119.24
1	A	73	HIS	C-N-CA	6.70	126.21	119.24
1	E	38	VAL	N-CA-C	6.62	115.18	107.77
1	B	31	HIS	N-CA-C	6.55	119.01	111.02
1	B	367	HIS	N-CA-C	-6.44	105.17	113.16
1	A	102	VAL	N-CA-C	6.38	117.89	108.45
1	E	308	ARG	N-CA-C	-6.37	104.78	112.54
1	E	102	VAL	N-CA-C	6.08	117.44	108.45
1	D	31	HIS	N-CA-C	6.07	118.42	111.02
1	D	308	ARG	N-CA-C	-6.00	105.22	112.54
1	E	101	HIS	N-CA-C	-5.84	101.84	110.48
1	A	38	VAL	N-CA-C	5.71	113.71	107.60
1	B	102	VAL	N-CA-C	5.66	116.83	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	MSE	N-CA-C	5.59	118.30	111.82
1	B	348	GLY	N-CA-C	-5.53	107.61	115.30
1	A	101	HIS	N-CA-C	-5.49	102.35	110.48
1	B	18	ILE	N-CA-C	5.45	117.17	108.89
1	B	366	GLY	N-CA-C	-5.42	105.73	113.86
1	B	101	HIS	N-CA-C	-5.31	102.61	110.48
1	D	113	GLN	N-CA-C	-5.24	105.47	111.07
1	A	261	ALA	N-CA-C	5.23	116.83	111.03
1	A	55	LYS	N-CA-C	5.17	117.66	111.71
1	D	332	LEU	N-CA-C	-5.12	105.78	111.36
1	D	73	HIS	CA-C-N	5.12	126.23	119.84
1	D	73	HIS	C-N-CA	5.12	126.23	119.84
1	A	279	ALA	N-CA-C	5.05	119.70	111.37
1	A	290	ILE	N-CA-C	5.05	115.24	108.17
1	D	38	VAL	N-CA-C	5.03	113.46	107.73
1	D	63	VAL	N-CA-C	5.00	114.38	106.32

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	2645	0	2618	71	0
1	B	2675	0	2646	61	0
1	D	2712	0	2685	74	0
1	E	2638	0	2595	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	210	0	0	2	0
3	B	181	0	0	3	0
3	D	118	0	0	4	0
3	E	175	0	0	3	0
All	All	11358	0	10544	248	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 12.

All (248) 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:361:ASN:HD22	1:E:364:ARG:HH12	1.08	0.98
1:A:101:HIS:HD2	1:A:128:LEU:H	1.12	0.97
1:A:224:HIS:CE1	1:B:224:HIS:HE1	1.82	0.96
1:A:224:HIS:HE1	1:B:224:HIS:CE1	1.84	0.96
1:D:224:HIS:HE1	1:E:224:HIS:HE1	0.98	0.95
1:B:349:MSE:HE3	1:B:350:VAL:H	1.32	0.94
1:D:228:ASN:HD21	1:E:209:ASN:HD21	1.14	0.91
1:A:150:GLN:HE22	1:A:300:GLN:HE22	1.16	0.90
1:D:224:HIS:CE1	1:E:224:HIS:HE1	1.89	0.89
1:A:224:HIS:HD2	1:A:237:HIS:HD2	1.21	0.86
1:D:224:HIS:HE1	1:E:224:HIS:CE1	1.89	0.86
1:D:222:TRP:HE1	1:E:158:HIS:HD2	1.24	0.85
1:A:158:HIS:HD2	1:B:222:TRP:HE1	1.24	0.84
1:E:361:ASN:ND2	1:E:364:ARG:HH12	1.79	0.80
1:D:146:GLN:O	1:D:150:GLN:HG3	1.80	0.79
1:B:349:MSE:HE3	1:B:350:VAL:N	1.98	0.78
1:A:146:GLN:HG2	1:A:150:GLN:HE21	1.49	0.77
1:A:224:HIS:CD2	1:A:237:HIS:HD2	2.02	0.77
1:B:184:LEU:HD12	1:B:188:LEU:HD12	1.67	0.77
1:E:224:HIS:HD2	1:E:237:HIS:HD2	1.30	0.76
1:D:171:ARG:NH1	1:D:173:ARG:HH21	1.82	0.76
1:A:366:GLY:C	1:A:368:HIS:H	1.94	0.75
1:D:285:ASP:HB3	3:D:481:HOH:O	1.86	0.75
1:B:327:PRO:HG2	1:B:330:GLU:HG3	1.66	0.75
1:D:224:HIS:HD2	1:D:237:HIS:ND1	1.85	0.74
1:D:241:LEU:HD13	1:E:157:LYS:HG3	1.70	0.73
1:D:327:PRO:HG2	1:D:330:GLU:HG3	1.70	0.73
1:E:134:ASN:HD22	1:E:307:GLN:NE2	1.86	0.73
1:E:309:GLN:HA	1:E:312:MSE:HE3	1.71	0.73
1:A:224:HIS:HD2	1:A:237:HIS:CD2	2.06	0.72
1:A:163:PHE:HE2	1:A:191:HIS:HB2	1.54	0.72
1:A:309:GLN:HA	1:A:312:MSE:HE3	1.71	0.72
1:E:361:ASN:HD22	1:E:364:ARG:NH1	1.87	0.72
1:B:163:PHE:CD2	1:B:188:LEU:HD13	2.26	0.70
1:D:97:ASN:HD22	1:D:125:LYS:HE2	1.57	0.69
1:D:32:ALA:HB3	1:D:33:PRO:HD3	1.74	0.69
1:A:101:HIS:CD2	1:A:128:LEU:H	2.03	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ARG:HB2	1:B:312:MSE:HE2	1.75	0.69
1:A:184:LEU:HD11	1:A:188:LEU:HD12	1.73	0.69
1:B:163:PHE:CE2	1:B:188:LEU:HD13	2.28	0.69
1:E:146:GLN:HE21	1:E:300:GLN:HE21	1.41	0.68
1:A:146:GLN:HG2	1:A:150:GLN:NE2	2.08	0.68
1:B:215:ASP:HA	3:B:524:HOH:O	1.92	0.68
1:B:32:ALA:HB3	1:B:33:PRO:HD3	1.73	0.68
1:B:119:ILE:HG12	1:B:328:PRO:HB2	1.75	0.68
1:A:32:ALA:HB3	1:A:33:PRO:HD3	1.76	0.67
1:E:224:HIS:CD2	1:E:237:HIS:HD2	2.10	0.67
1:B:309:GLN:HA	1:B:312:MSE:HE3	1.77	0.67
1:D:146:GLN:HE21	1:D:150:GLN:NE2	1.94	0.65
1:B:113:GLN:O	1:B:117:GLU:HG3	1.97	0.65
1:E:224:HIS:HD2	1:E:237:HIS:CD2	2.12	0.65
1:E:258:VAL:C	1:E:259:ILE:HD12	2.22	0.64
1:B:342:VAL:O	1:B:346:GLU:HG3	1.98	0.64
1:B:145:ARG:HD3	3:B:467:HOH:O	1.97	0.63
1:E:119:ILE:HG12	1:E:328:PRO:HB2	1.81	0.63
1:A:309:GLN:CA	1:A:312:MSE:HE3	2.29	0.63
1:D:252:HIS:HD2	1:D:257:SER:OG	1.79	0.63
1:D:255:LYS:HE3	3:D:406:HOH:O	1.99	0.62
1:B:224:HIS:HD2	1:B:237:HIS:ND1	1.97	0.62
1:E:32:ALA:O	1:E:36:ARG:HG3	2.00	0.62
1:D:291:TYR:CD1	1:D:297:ALA:HB2	2.35	0.62
1:E:163:PHE:CD2	1:E:188:LEU:HD22	2.35	0.61
1:B:308:ARG:CB	1:B:312:MSE:HE2	2.31	0.60
1:A:119:ILE:HG12	1:A:328:PRO:HB2	1.83	0.60
1:A:308:ARG:HB2	1:A:312:MSE:HE2	1.82	0.60
1:D:97:ASN:HD21	1:D:121:LEU:HD11	1.67	0.60
1:D:171:ARG:HH11	1:D:173:ARG:HH21	1.46	0.60
1:A:150:GLN:HE22	1:A:300:GLN:NE2	1.94	0.59
1:B:28:LYS:HE2	1:B:57:ASP:OD2	2.02	0.59
1:E:13:ASN:O	1:E:14:ASN:HB2	2.01	0.59
1:D:365:GLU:HG3	1:D:366:GLY:N	2.17	0.59
1:A:58:LEU:O	1:A:61:VAL:HG22	2.03	0.59
1:E:128:LEU:C	1:E:128:LEU:HD23	2.27	0.59
1:D:113:GLN:O	1:D:117:GLU:HG3	2.03	0.58
1:B:68:GLU:CD	1:B:68:GLU:H	2.11	0.58
1:E:134:ASN:HD22	1:E:307:GLN:HE22	1.50	0.58
1:B:309:GLN:CA	1:B:312:MSE:HE3	2.34	0.58
1:E:135:ARG:HG3	1:E:191:HIS:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:TYR:CE1	1:B:297:ALA:HB2	2.40	0.57
1:A:348:GLY:O	1:B:349:MSE:HE3	2.04	0.57
1:A:366:GLY:C	1:A:368:HIS:N	2.63	0.57
1:E:129:LEU:O	1:E:328:PRO:HD3	2.04	0.57
1:B:258:VAL:C	1:B:259:ILE:HD12	2.30	0.57
1:A:308:ARG:CB	1:A:312:MSE:HE2	2.35	0.57
1:A:361:ASN:OD1	1:A:364:ARG:NH2	2.37	0.57
1:B:11:LEU:HD11	1:B:42:ASN:ND2	2.20	0.56
1:B:93:ARG:NH1	3:B:519:HOH:O	2.37	0.56
1:E:309:GLN:CA	1:E:312:MSE:HE3	2.34	0.56
1:E:342:VAL:O	1:E:346:GLU:HG2	2.04	0.56
1:A:224:HIS:CE1	1:B:224:HIS:CE1	2.72	0.56
1:A:366:GLY:O	1:A:368:HIS:N	2.39	0.56
1:A:87:THR:C	1:A:90:PRO:HD2	2.30	0.56
1:B:191:HIS:CE1	1:B:192:LEU:HD13	2.41	0.55
1:B:365:GLU:OE1	1:D:60:ASP:HB3	2.05	0.55
1:A:163:PHE:HB3	1:A:188:LEU:HD13	1.87	0.55
1:A:258:VAL:C	1:A:259:ILE:HD12	2.32	0.55
1:A:309:GLN:N	1:A:312:MSE:HE3	2.21	0.55
1:B:11:LEU:HD11	1:B:42:ASN:HD21	1.71	0.55
1:B:184:LEU:CD1	1:B:188:LEU:HD12	2.37	0.55
1:B:308:ARG:O	1:B:312:MSE:HG3	2.06	0.55
1:D:85:ASN:HB3	1:D:110:LEU:HD21	1.90	0.54
1:E:361:ASN:HA	1:E:364:ARG:NH1	2.22	0.54
1:A:47:ALA:HA	1:A:64:ILE:O	2.08	0.54
1:A:145:ARG:O	1:A:149:GLU:HG3	2.08	0.54
1:E:32:ALA:HB3	1:E:33:PRO:HD3	1.90	0.54
1:A:119:ILE:O	1:A:123:GLU:HG3	2.08	0.54
1:E:58:LEU:O	1:E:61:VAL:HG12	2.07	0.54
1:B:277:GLY:H	1:B:281:TRP:CG	2.26	0.53
1:D:309:GLN:HE21	1:D:309:GLN:HA	1.74	0.53
1:E:163:PHE:CG	1:E:188:LEU:HD22	2.42	0.53
1:A:129:LEU:O	1:A:328:PRO:HD3	2.07	0.53
1:E:308:ARG:HB2	1:E:312:MSE:HE2	1.90	0.53
1:D:171:ARG:NH1	1:D:173:ARG:NH2	2.55	0.53
1:A:153:LEU:HD12	1:A:153:LEU:H	1.74	0.52
1:A:184:LEU:HD11	1:A:188:LEU:CD1	2.38	0.52
1:A:319:LYS:HE2	1:A:321:GLN:NE2	2.25	0.52
1:D:97:ASN:ND2	1:D:121:LEU:HD11	2.24	0.52
1:D:21:ILE:HA	1:D:47:ALA:HB3	1.91	0.52
1:E:259:ILE:HD12	1:E:259:ILE:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:SER:C	1:D:296:GLN:H	2.17	0.52
1:A:248:ARG:HD3	1:A:263:ALA:HB2	1.92	0.51
1:A:97:ASN:HD22	1:A:125:LYS:HE3	1.75	0.51
1:B:129:LEU:O	1:B:328:PRO:HD3	2.11	0.51
1:A:93:ARG:HD2	3:A:513:HOH:O	2.10	0.51
1:B:309:GLN:N	1:B:312:MSE:HE3	2.27	0.50
1:D:83:SER:HB2	1:D:84:PRO:HD2	1.94	0.50
1:A:128:LEU:HD23	1:A:128:LEU:C	2.37	0.50
1:B:119:ILE:O	1:B:123:GLU:HG3	2.11	0.50
1:B:169:GLU:CD	1:B:169:GLU:H	2.20	0.50
1:D:119:ILE:HG12	1:D:328:PRO:HB2	1.94	0.50
1:D:224:HIS:CE1	1:E:224:HIS:CE1	2.79	0.50
1:A:165:ARG:HH11	1:A:167:ARG:NH2	2.10	0.50
1:D:202:LEU:HD11	1:D:363:LEU:HD12	1.94	0.50
1:E:308:ARG:CB	1:E:312:MSE:HE2	2.42	0.50
1:E:298:HIS:HD2	3:E:520:HOH:O	1.94	0.49
1:D:97:ASN:ND2	1:D:125:LYS:HE2	2.24	0.49
1:A:349:MSE:HE3	1:A:350:VAL:HB	1.93	0.49
1:A:245:GLY:HA3	1:B:259:ILE:HD11	1.94	0.49
1:A:348:GLY:O	1:B:349:MSE:CE	2.60	0.49
1:A:260:LYS:HD3	1:A:288:LEU:HD23	1.93	0.49
1:D:107:PRO:O	1:D:108:PHE:C	2.55	0.49
1:E:277:GLY:H	1:E:281:TRP:CG	2.31	0.49
1:B:83:SER:HB2	1:B:84:PRO:CD	2.43	0.49
1:A:45:PHE:CD1	1:A:62:THR:HB	2.48	0.48
1:B:47:ALA:HA	1:B:64:ILE:O	2.13	0.48
1:E:364:ARG:NH1	1:E:364:ARG:HB3	2.28	0.48
1:B:101:HIS:CE1	1:B:127:ARG:HH11	2.31	0.48
1:B:135:ARG:HG3	1:B:191:HIS:HB2	1.96	0.48
1:D:228:ASN:ND2	1:E:209:ASN:HD21	1.97	0.48
1:D:97:ASN:ND2	1:D:121:LEU:HD21	2.28	0.48
1:E:163:PHE:CE2	1:E:188:LEU:HD22	2.49	0.48
1:B:57:ASP:C	1:B:59:PRO:HD3	2.39	0.48
1:D:153:LEU:O	1:D:253:GLY:HA3	2.14	0.48
1:A:277:GLY:H	1:A:281:TRP:CG	2.32	0.48
1:E:361:ASN:HA	1:E:364:ARG:HH12	1.79	0.47
1:D:291:TYR:CE1	1:D:297:ALA:HB2	2.48	0.47
1:A:89:ALA:HB3	1:A:90:PRO:HD3	1.96	0.47
1:B:150:GLN:HE22	1:B:300:GLN:HE22	1.61	0.47
1:D:129:LEU:O	1:D:328:PRO:HD3	2.14	0.47
1:E:146:GLN:O	1:E:150:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:LEU:C	1:D:128:LEU:HD23	2.39	0.47
1:A:51:GLU:HG3	1:A:63:VAL:HG21	1.97	0.47
1:A:148:ILE:HA	1:A:153:LEU:HD11	1.97	0.47
1:B:277:GLY:H	1:B:281:TRP:CD1	2.32	0.47
1:D:83:SER:HB2	1:D:84:PRO:CD	2.45	0.47
1:D:145:ARG:HD2	3:D:472:HOH:O	2.14	0.47
1:E:361:ASN:O	1:E:365:GLU:HG3	2.14	0.47
1:A:83:SER:HB2	1:A:84:PRO:CD	2.44	0.47
1:D:146:GLN:HE21	1:D:150:GLN:HE21	1.63	0.47
1:E:37:SER:OG	1:E:308:ARG:HD2	2.15	0.46
1:E:291:TYR:CE1	1:E:297:ALA:HB2	2.51	0.46
1:D:357:ASP:OD2	1:D:357:ASP:N	2.49	0.46
1:E:146:GLN:HE21	1:E:300:GLN:NE2	2.11	0.46
1:A:191:HIS:CG	3:A:404:HOH:O	2.69	0.46
1:E:47:ALA:HA	1:E:64:ILE:O	2.15	0.46
1:B:83:SER:HB2	1:B:84:PRO:HD2	1.97	0.46
1:E:81:ILE:O	1:E:105:ASP:HB2	2.16	0.46
1:A:93:ARG:HG3	1:A:118:LEU:HD21	1.97	0.46
1:D:224:HIS:CD2	1:D:237:HIS:ND1	2.75	0.46
1:D:64:ILE:HG22	1:D:66:SER:H	1.81	0.46
1:D:222:TRP:HE1	1:E:158:HIS:CD2	2.16	0.45
1:B:259:ILE:HD12	1:B:259:ILE:N	2.32	0.45
1:A:277:GLY:H	1:A:281:TRP:CD1	2.35	0.45
1:D:227:LEU:HB2	1:D:234:VAL:HB	1.98	0.45
1:D:310:TYR:O	1:D:314:ILE:HG12	2.16	0.45
1:D:185:TRP:CE2	1:D:338:LEU:HD12	2.52	0.45
1:D:293:ALA:O	1:D:294:SER:HB3	2.17	0.45
1:D:144:ILE:HD13	1:D:144:ILE:HA	1.87	0.44
1:A:162:HIS:O	1:A:248:ARG:HD2	2.17	0.44
1:D:113:GLN:HA	1:D:113:GLN:HE21	1.82	0.44
1:D:73:HIS:ND1	1:D:74:PRO:HD2	2.33	0.44
1:E:113:GLN:NE2	3:E:423:HOH:O	2.49	0.44
1:E:309:GLN:N	1:E:312:MSE:HE3	2.33	0.44
1:D:294:SER:C	1:D:296:GLN:N	2.76	0.44
1:E:356:SER:OG	1:E:359:GLU:HG3	2.18	0.44
1:A:73:HIS:ND1	1:A:74:PRO:HD2	2.32	0.44
1:A:152:THR:HG21	1:A:290:ILE:HG21	2.00	0.44
1:E:361:ASN:ND2	1:E:364:ARG:HH22	2.16	0.44
1:A:252:HIS:CE1	1:B:242:VAL:HG13	2.53	0.43
1:B:97:ASN:HD22	1:B:125:LYS:HE3	1.82	0.43
1:B:66:SER:HA	1:B:67:PRO:HD3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:LEU:HB2	1:E:234:VAL:HB	1.99	0.43
1:A:290:ILE:O	1:A:297:ALA:HA	2.18	0.43
1:D:163:PHE:CD2	1:D:188:LEU:HG	2.53	0.43
1:B:128:LEU:C	1:B:128:LEU:HD23	2.44	0.43
1:A:259:ILE:HD12	1:A:259:ILE:N	2.32	0.43
1:D:85:ASN:CB	1:D:110:LEU:HD21	2.49	0.43
1:B:290:ILE:O	1:B:297:ALA:HA	2.17	0.43
1:D:73:HIS:CG	1:D:74:PRO:HD2	2.54	0.43
1:D:187:ASP:C	1:D:188:LEU:HD22	2.44	0.43
1:A:169:GLU:CD	1:A:169:GLU:H	2.26	0.42
1:E:13:ASN:HB3	1:E:14:ASN:H	1.38	0.42
1:D:183:GLY:CA	1:D:219:ILE:HG12	2.49	0.42
1:E:146:GLN:NE2	1:E:300:GLN:HE21	2.12	0.42
1:A:361:ASN:O	1:A:365:GLU:HG2	2.20	0.42
1:D:61:VAL:HG23	1:D:61:VAL:O	2.19	0.42
1:A:73:HIS:HA	1:A:74:PRO:HD3	1.86	0.42
1:D:367:HIS:O	1:D:368:HIS:HB2	2.19	0.42
1:A:87:THR:O	1:A:90:PRO:HD2	2.19	0.42
1:A:158:HIS:CD2	1:B:222:TRP:HE1	2.16	0.42
1:D:249:PHE:HB2	1:D:260:LYS:HB3	2.01	0.42
1:D:365:GLU:HG3	1:D:366:GLY:H	1.85	0.42
1:A:291:TYR:CE1	1:A:297:ALA:HB2	2.55	0.42
1:D:163:PHE:CE2	1:D:188:LEU:HG	2.54	0.42
1:D:295:LEU:HD23	1:D:295:LEU:N	2.35	0.42
1:A:71:VAL:HG23	1:A:72:GLN:HG3	2.01	0.42
1:A:83:SER:HB2	1:A:84:PRO:HD2	2.01	0.42
1:D:160:GLU:HB3	1:D:250:THR:HB	2.02	0.42
1:D:228:ASN:HD21	1:E:209:ASN:ND2	1.97	0.42
1:E:31:HIS:HE2	1:E:105:ASP:CG	2.27	0.42
1:E:214:ARG:NH2	3:E:511:HOH:O	2.50	0.42
1:B:71:VAL:CG1	1:B:95:ALA:HA	2.49	0.41
1:B:157:LYS:HD3	1:B:157:LYS:HA	1.85	0.41
1:D:18:ILE:HG22	1:D:19:ALA:N	2.33	0.41
1:B:68:GLU:CD	1:B:68:GLU:N	2.78	0.41
1:E:46:VAL:HG23	1:E:61:VAL:HG21	2.02	0.41
1:E:89:ALA:HB3	1:E:90:PRO:CD	2.50	0.41
1:A:73:HIS:HB3	1:A:76:VAL:HG23	2.01	0.41
1:D:144:ILE:HG13	1:D:249:PHE:CG	2.55	0.41
1:E:290:ILE:O	1:E:297:ALA:HA	2.20	0.41
1:D:296:GLN:OE1	1:D:296:GLN:HA	2.21	0.41
1:B:57:ASP:O	1:B:59:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ARG:HG3	1:B:191:HIS:CB	2.51	0.40
1:D:128:LEU:HD13	1:D:318:LEU:HD13	2.02	0.40
1:D:233:LYS:HE2	3:D:401:HOH:O	2.21	0.40
1:E:145:ARG:O	1:E:149:GLU:HG3	2.21	0.40
1:B:191:HIS:NE2	1:B:192:LEU:HD13	2.37	0.40
1:D:140:ASP:OD1	1:D:141:TYR:N	2.54	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	339/364 (93%)	331 (98%)	7 (2%)	1 (0%)	36	30
1	B	343/364 (94%)	334 (97%)	9 (3%)	0	100	100
1	D	346/364 (95%)	328 (95%)	16 (5%)	2 (1%)	21	13
1	E	340/364 (93%)	329 (97%)	10 (3%)	1 (0%)	36	30
All	All	1368/1456 (94%)	1322 (97%)	42 (3%)	4 (0%)	36	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	294	SER
1	E	14	ASN
1	A	367	HIS
1	D	74	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	280/294 (95%)	278 (99%)	2 (1%)	76	80
1	B	284/294 (97%)	280 (99%)	4 (1%)	59	60
1	D	286/294 (97%)	282 (99%)	4 (1%)	59	60
1	E	278/294 (95%)	276 (99%)	2 (1%)	76	80
All	All	1128/1176 (96%)	1116 (99%)	12 (1%)	65	68

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	LEU
1	A	169	GLU
1	B	169	GLU
1	B	192	LEU
1	B	219	ILE
1	B	265	GLN
1	D	124	GLU
1	D	153	LEU
1	D	309	GLN
1	D	318	LEU
1	E	105	ASP
1	E	215	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	72	GLN
1	A	97	ASN
1	A	101	HIS
1	A	146	GLN
1	A	150	GLN
1	A	158	HIS
1	A	204	GLN
1	A	224	HIS
1	A	237	HIS
1	A	283	GLN

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Mol	Chain	Res	Type
1	A	304	GLN
1	A	321	GLN
1	B	42	ASN
1	B	97	ASN
1	B	146	GLN
1	B	224	HIS
1	B	265	GLN
1	B	283	GLN
1	B	298	HIS
1	B	300	GLN
1	D	17	ASN
1	D	97	ASN
1	D	113	GLN
1	D	146	GLN
1	D	224	HIS
1	D	228	ASN
1	D	252	HIS
1	D	265	GLN
1	D	298	HIS
1	D	300	GLN
1	D	309	GLN
1	D	321	GLN
1	E	72	GLN
1	E	97	ASN
1	E	113	GLN
1	E	146	GLN
1	E	158	HIS
1	E	204	GLN
1	E	224	HIS
1	E	237	HIS
1	E	298	HIS
1	E	304	GLN
1	E	307	GLN
1	E	361	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [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	338/364 (92%)	-0.13	5 (1%) 72 73	14, 24, 39, 50	0
1	B	342/364 (93%)	-0.02	11 (3%) 50 50	14, 24, 40, 57	0
1	D	345/364 (94%)	0.63	28 (8%) 18 18	16, 33, 49, 59	0
1	E	339/364 (93%)	0.08	10 (2%) 53 55	15, 27, 41, 52	0
All	All	1364/1456 (93%)	0.14	54 (3%) 42 42	14, 27, 46, 59	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	HIS	4.4
1	D	60	ASP	4.4
1	E	13	ASN	4.3
1	D	368	HIS	4.1
1	B	365	GLU	3.9
1	E	368	HIS	3.9
1	D	295	LEU	3.6
1	D	113	GLN	3.5
1	E	219	ILE	3.5
1	D	293	ALA	3.4
1	D	86	ALA	3.3
1	D	110	LEU	3.2
1	D	356	SER	3.1
1	B	368	HIS	3.1
1	D	360	ARG	3.1
1	D	117	GLU	3.0
1	A	169	GLU	2.9
1	E	218	GLU	2.8
1	B	366	GLY	2.8
1	D	63	VAL	2.7
1	B	169	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	278	SER	2.7
1	D	153	LEU	2.7
1	D	365	GLU	2.6
1	B	62	THR	2.6
1	D	361	ASN	2.5
1	D	169	GLU	2.5
1	D	358	ASP	2.5
1	E	14	ASN	2.4
1	B	215	ASP	2.4
1	B	170	VAL	2.4
1	E	215	ASP	2.4
1	D	230	PRO	2.4
1	D	58	LEU	2.3
1	A	163	PHE	2.3
1	D	357	ASP	2.3
1	D	75	ASP	2.3
1	A	153	LEU	2.3
1	B	182	SER	2.2
1	B	216	GLY	2.2
1	D	44	ALA	2.2
1	E	56	ARG	2.2
1	A	170	VAL	2.2
1	D	64	ILE	2.1
1	E	216	GLY	2.1
1	B	11	LEU	2.1
1	D	59	PRO	2.1
1	D	367	HIS	2.1
1	E	217	ALA	2.1
1	D	61	VAL	2.0
1	E	182	SER	2.0
1	D	299	ALA	2.0
1	D	126	GLN	2.0
1	B	367	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

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(Å ²)	Q<0.9
2	CL	D	3	1/1	0.96	0.10	37,37,37,37	0
2	CL	E	4	1/1	0.97	0.07	36,36,36,36	0
2	CL	A	1	1/1	0.99	0.05	24,24,24,24	0
2	CL	B	2	1/1	0.99	0.05	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.