Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2025 – 08:14 PM JST

PDB ID	:	8YXS
Title	:	X-ray structure of non-heme iron dioxygenase from Aspergillus brunneoviolaceus
Authors	:	Lv, X.; Ma, X.
Deposited on	:	2024-04-02
Resolution	:	3.62 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:

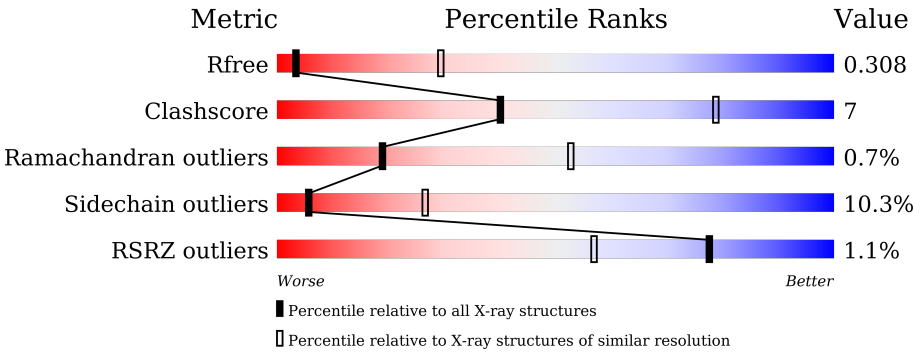
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

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 3.62 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}	164625	1619 (3.74-3.50)
Clashscore	180529	1721 (3.74-3.50)
Ramachandran outliers	177936	1694 (3.74-3.50)
Sidechain outliers	177891	1693 (3.74-3.50)
RSRZ outliers	164620	1618 (3.74-3.50)

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	456	73% 23%
1	B	456	77% 20%
1	C	456	71% 24%
1	D	456	73% 23%
1	E	456	78% 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17736 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 Oxidoreductase AflY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total 3546	C 2250	N 630	O 649	S 17	0	0	0
1	B	446	Total 3546	C 2250	N 630	O 649	S 17	0	0	0
1	C	446	Total 3546	C 2250	N 630	O 649	S 17	0	0	0
1	D	446	Total 3546	C 2250	N 630	O 649	S 17	0	0	0
1	E	446	Total 3546	C 2250	N 630	O 649	S 17	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	VAL	ALA	conflict	UNP A0A8G1RKM4
A	251	VAL	LEU	conflict	UNP A0A8G1RKM4
A	441	MET	ASN	engineered mutation	UNP A0A8G1RKM4
B	31	VAL	ALA	conflict	UNP A0A8G1RKM4
B	251	VAL	LEU	conflict	UNP A0A8G1RKM4
B	441	MET	ASN	engineered mutation	UNP A0A8G1RKM4
C	31	VAL	ALA	conflict	UNP A0A8G1RKM4
C	251	VAL	LEU	conflict	UNP A0A8G1RKM4
C	441	MET	ASN	engineered mutation	UNP A0A8G1RKM4
D	31	VAL	ALA	conflict	UNP A0A8G1RKM4
D	251	VAL	LEU	conflict	UNP A0A8G1RKM4
D	441	MET	ASN	engineered mutation	UNP A0A8G1RKM4
E	31	VAL	ALA	conflict	UNP A0A8G1RKM4
E	251	VAL	LEU	conflict	UNP A0A8G1RKM4
E	441	MET	ASN	engineered mutation	UNP A0A8G1RKM4

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 3 is water.

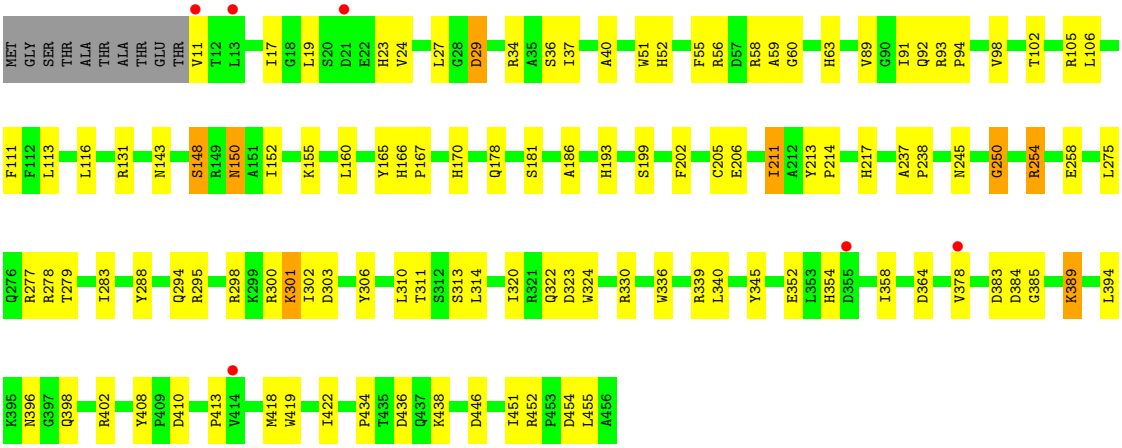
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0

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.

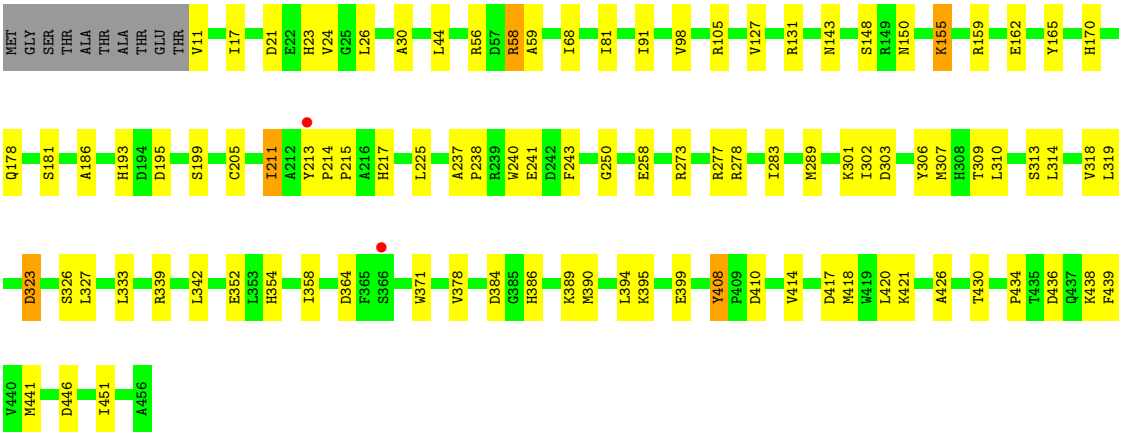
• Molecule 1: Oxidoreductase AflY

Chain A:



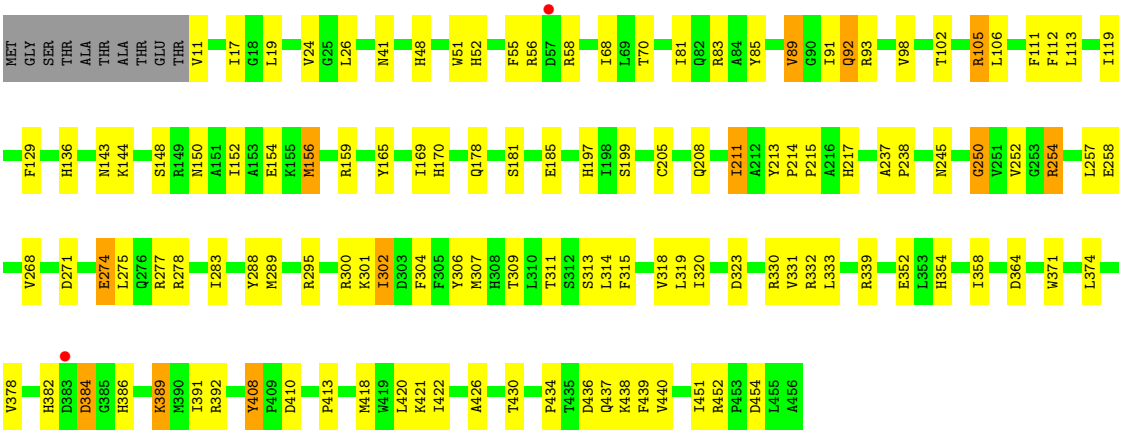
• Molecule 1: Oxidoreductase AflY

Chain B:



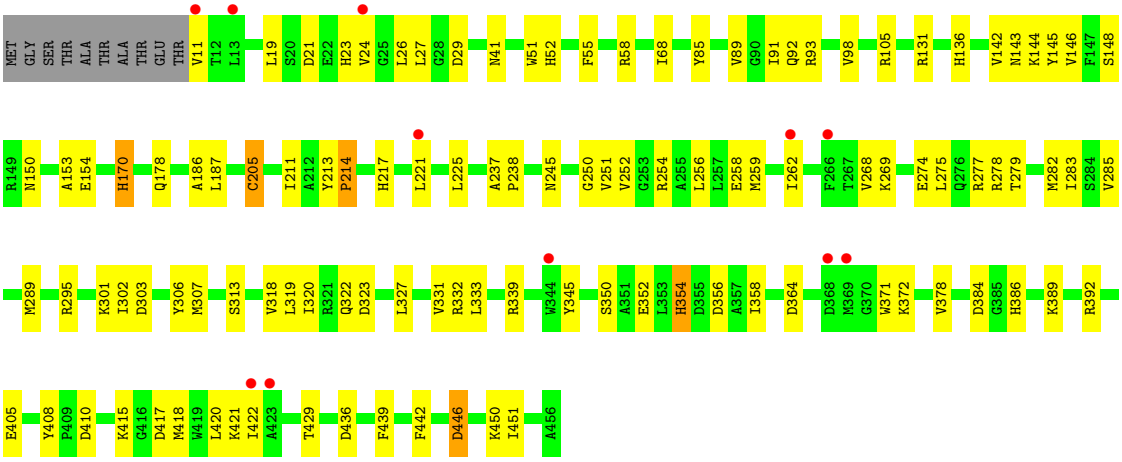
• Molecule 1: Oxidoreductase AflY

Chain C:



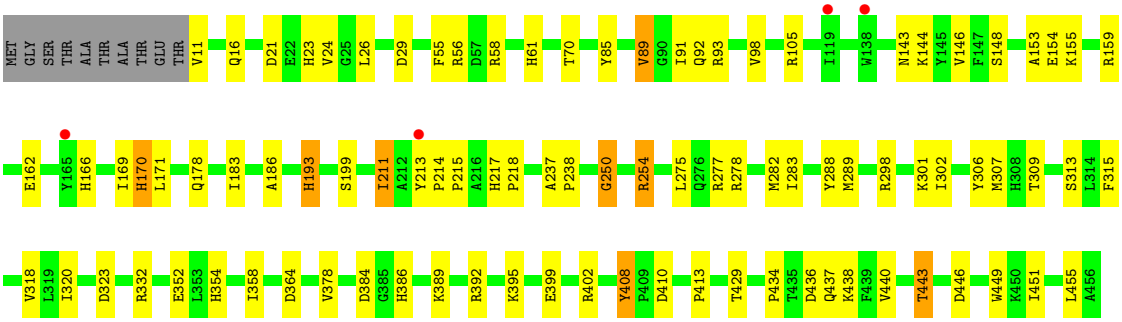
• Molecule 1: Oxidoreductase AflY

Chain D:



• Molecule 1: Oxidoreductase AflY

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	256.99Å 109.74Å 179.89Å 90.00° 93.39° 90.00°	Depositor
Resolution (Å)	71.59 – 3.62 71.59 – 3.62	Depositor EDS
% Data completeness (in resolution range)	99.8 (71.59-3.62) 99.7 (71.59-3.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.276 , 0.312 0.278 , 0.308	Depositor DCC
R_{free} test set	2888 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	99.2	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	17736	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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

5.1 Standard geometry

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

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	0.28	0/3620	0.49	0/4902
1	B	0.27	0/3620	0.48	0/4902
1	C	0.25	0/3620	0.47	0/4902
1	D	0.27	0/3620	0.47	0/4902
1	E	0.26	0/3620	0.47	0/4902
All	All	0.27	0/18100	0.48	0/24510

There are no bond length outliers.

There are no bond angle outliers.

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	3546	0	3451	53	0
1	B	3546	0	3451	41	0
1	C	3546	0	3451	60	0
1	D	3546	0	3451	45	0
1	E	3546	0	3451	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	1	0	0	2	0
All	All	17736	0	17255	228	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 7.

All (228) 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:C:434:PRO:HD2	1:C:437:GLN:HB2	1.64	0.78
1:D:283:ILE:HG12	1:D:313:SER:HB2	1.68	0.76
1:D:252:VAL:HG13	1:D:256:LEU:HD13	1.70	0.71
1:A:63:HIS:CE1	3:A:601:HOH:O	2.44	0.70
1:B:283:ILE:HG12	1:B:313:SER:HB2	1.72	0.70
1:A:283:ILE:HG12	1:A:313:SER:HB2	1.74	0.69
1:E:283:ILE:HG12	1:E:313:SER:HB2	1.75	0.69
1:A:166:HIS:CE1	3:A:601:HOH:O	2.46	0.68
1:C:283:ILE:HG12	1:C:313:SER:HB2	1.76	0.67
1:C:275:LEU:HD21	1:C:320:ILE:HB	1.77	0.67
1:C:384:ASP:OD1	1:C:386:HIS:ND1	2.28	0.66
1:B:319:LEU:HD13	1:B:333:LEU:HD13	1.78	0.65
1:B:26:LEU:HD13	1:B:318:VAL:HG22	1.79	0.65
1:A:258:GLU:N	1:A:258:GLU:OE1	2.31	0.63
1:A:402:ARG:HH12	1:B:273:ARG:HE	1.47	0.63
1:B:148:SER:OG	1:B:150:ASN:ND2	2.25	0.63
1:D:269:LYS:HB2	1:D:274:GLU:HG2	1.80	0.62
1:D:319:LEU:HD13	1:D:333:LEU:HD13	1.81	0.62
1:D:275:LEU:HD21	1:D:320:ILE:HB	1.80	0.61
1:E:144:LYS:HA	1:E:148:SER:HB3	1.82	0.61
1:C:302:ILE:HB	1:C:439:PHE:HD2	1.65	0.61
1:C:148:SER:OG	1:C:150:ASN:ND2	2.34	0.61
1:E:298:ARG:NH1	1:E:455:LEU:O	2.34	0.60
1:C:258:GLU:N	1:C:258:GLU:OE1	2.34	0.60
1:D:301:LYS:HD3	1:D:429:THR:HB	1.84	0.60
1:E:159:ARG:NH1	1:E:193:HIS:O	2.33	0.60
1:A:303:ASP:OD2	1:A:306:TYR:N	2.34	0.59
1:A:55:PHE:HA	1:A:93:ARG:HG2	1.83	0.59
1:C:154:GLU:OE1	1:C:332:ARG:NH2	2.35	0.58
1:E:55:PHE:HA	1:E:93:ARG:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:MET:HE1	1:E:386:HIS:HB3	1.85	0.58
1:B:170:HIS:HB3	1:B:186:ALA:HB2	1.86	0.58
1:C:105:ARG:HB3	1:C:111:PHE:CG	2.38	0.58
1:D:148:SER:HG	1:D:150:ASN:HD22	1.49	0.58
1:C:271:ASP:HB3	1:C:274:GLU:HB3	1.85	0.57
1:A:34:ARG:HH11	1:B:30:ALA:HA	1.70	0.57
1:D:154:GLU:OE1	1:D:332:ARG:NH2	2.38	0.57
1:D:170:HIS:HB3	1:D:186:ALA:HB2	1.87	0.57
1:A:102:THR:HG23	1:A:111:PHE:HE2	1.70	0.57
1:B:56:ARG:NH2	1:B:58:ARG:O	2.38	0.56
1:C:452:ARG:NH2	1:C:454:ASP:OD2	2.38	0.56
1:D:268:VAL:HB	1:D:331:VAL:HG13	1.87	0.56
1:C:268:VAL:HB	1:C:331:VAL:HG13	1.88	0.56
1:B:441:MET:HE1	1:C:211:ILE:HB	1.88	0.55
1:D:19:LEU:H	1:D:41:ASN:HD21	1.54	0.55
1:B:148:SER:HG	1:B:150:ASN:HD22	1.50	0.55
1:C:55:PHE:HA	1:C:93:ARG:HG2	1.88	0.55
1:B:258:GLU:OE1	1:B:258:GLU:N	2.35	0.55
1:E:275:LEU:HD21	1:E:320:ILE:HB	1.88	0.55
1:D:225:LEU:HD11	1:D:285:VAL:HG13	1.89	0.54
1:D:142:VAL:HG22	1:D:187:LEU:HD11	1.89	0.54
1:B:277:ARG:NH2	1:B:278:ARG:HD3	2.23	0.54
1:B:371:TRP:CE2	1:B:420:LEU:HD13	2.42	0.54
1:A:160:LEU:HA	1:A:167:PRO:HB2	1.90	0.53
1:A:298:ARG:NH1	1:A:455:LEU:O	2.42	0.53
1:D:55:PHE:HA	1:D:93:ARG:HG2	1.89	0.53
1:B:240:TRP:HD1	1:C:257:LEU:HD22	1.73	0.53
1:D:277:ARG:NH2	1:D:278:ARG:HD3	2.24	0.53
1:A:303:ASP:HB3	1:A:306:TYR:HB2	1.91	0.53
1:C:55:PHE:CE2	1:C:56:ARG:HG3	2.44	0.52
1:A:322:GLN:OE1	1:A:324:TRP:NE1	2.37	0.52
1:B:302:ILE:HB	1:B:439:PHE:HD2	1.73	0.52
1:A:170:HIS:HB3	1:A:186:ALA:HB2	1.90	0.52
1:C:85:TYR:O	1:C:89:VAL:HB	2.08	0.52
1:A:27:LEU:HD21	1:A:396:ASN:HB2	1.90	0.52
1:A:36:SER:O	1:A:40:ALA:N	2.40	0.52
1:A:306:TYR:HE1	1:A:345:TYR:HA	1.74	0.52
1:C:26:LEU:HD13	1:C:318:VAL:HG22	1.91	0.52
1:B:68:ILE:HG23	1:B:81:ILE:HG23	1.91	0.51
1:A:51:TRP:HB3	1:A:92:GLN:HG3	1.93	0.51
1:C:165:TYR:HE2	1:C:309:THR:HG22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:GLU:N	1:D:258:GLU:OE1	2.43	0.51
1:D:148:SER:HG	1:D:150:ASN:ND2	2.08	0.51
1:D:303:ASP:HB3	1:D:306:TYR:HB2	1.93	0.51
1:C:169:ILE:HG12	1:C:315:PHE:CD2	2.46	0.51
1:B:414:VAL:HG13	1:B:418:MET:HB2	1.92	0.51
1:A:452:ARG:NH2	1:A:454:ASP:OD2	2.44	0.51
1:E:434:PRO:HD2	1:E:437:GLN:HB2	1.93	0.50
1:D:306:TYR:CE1	1:D:345:TYR:HA	2.47	0.50
1:E:154:GLU:OE1	1:E:332:ARG:NH2	2.44	0.50
1:B:241:GLU:HG3	1:C:257:LEU:HD21	1.94	0.50
1:E:306:TYR:O	1:E:309:THR:OG1	2.22	0.50
1:A:294:GLN:HG3	1:A:300:ARG:HG3	1.94	0.49
1:C:371:TRP:CE2	1:C:420:LEU:HD13	2.47	0.49
1:C:197:HIS:HB3	1:C:252:VAL:HG11	1.94	0.49
1:C:144:LYS:HA	1:C:148:SER:HB3	1.94	0.48
1:C:311:THR:HB	1:C:389:KCX:HG3	1.95	0.48
1:C:105:ARG:HB3	1:C:111:PHE:CD2	2.48	0.48
1:C:17:ILE:HG12	1:C:181:SER:OG	2.14	0.48
1:B:307:MET:HE2	1:B:390:MET:HG3	1.95	0.48
1:C:426:ALA:O	1:C:430:THR:OG1	2.16	0.48
1:E:395:LYS:O	1:E:399:GLU:HG2	2.14	0.48
1:B:165:TYR:HE2	1:B:309:THR:HG22	1.79	0.48
1:C:211:ILE:O	1:C:213:TYR:HD1	1.96	0.48
1:A:113:LEU:HD21	1:A:152:ILE:HG12	1.96	0.47
1:D:302:ILE:HB	1:D:439:PHE:HD2	1.78	0.47
1:C:319:LEU:HD13	1:C:333:LEU:HD13	1.96	0.47
1:A:148:SER:HG	1:A:150:ASN:HD22	1.62	0.47
1:A:383:ASP:CG	1:A:385:GLY:H	2.18	0.47
1:D:405:GLU:HG2	1:D:415:LYS:HG2	1.96	0.47
1:A:165:TYR:CE1	1:A:340:LEU:HD23	2.50	0.47
1:E:169:ILE:HG12	1:E:315:PHE:CD2	2.50	0.47
1:E:277:ARG:NH2	1:E:278:ARG:HD3	2.30	0.47
1:B:303:ASP:HB3	1:B:306:TYR:HB2	1.97	0.47
1:E:237:ALA:HB3	1:E:238:PRO:HD3	1.97	0.47
1:C:19:LEU:HB2	1:C:41:ASN:HD21	1.80	0.47
1:A:211:ILE:O	1:A:213:TYR:HD1	1.98	0.46
1:D:259:MET:HE3	1:D:262:ILE:HB	1.95	0.46
1:E:170:HIS:HB3	1:E:186:ALA:HB2	1.97	0.46
1:E:399:GLU:OE1	1:E:402:ARG:NH2	2.49	0.46
1:B:277:ARG:HD2	1:B:408:TYR:CE2	2.50	0.46
1:C:70:THR:HG23	1:C:392:ARG:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ARG:HE	1:C:382:HIS:HA	1.80	0.46
1:B:211:ILE:H	1:B:211:ILE:HG13	1.33	0.46
1:C:208:GLN:HA	1:C:211:ILE:HG13	1.98	0.46
1:C:156:MET:HA	1:C:159:ARG:HB2	1.97	0.46
1:D:237:ALA:HB3	1:D:238:PRO:HD3	1.97	0.46
1:E:301:LYS:HG2	1:E:440:VAL:HG23	1.98	0.46
1:E:70:THR:HG23	1:E:392:ARG:HD3	1.98	0.46
1:A:55:PHE:CE1	1:A:60:GLY:HA2	2.51	0.46
1:A:311:THR:HB	1:A:389:KCX:HG3	1.98	0.46
1:B:211:ILE:O	1:B:213:TYR:HD1	1.99	0.46
1:C:374:LEU:HB3	1:C:391:ILE:HD13	1.98	0.46
1:A:275:LEU:HD21	1:A:320:ILE:HB	1.97	0.45
1:E:278:ARG:HA	1:E:278:ARG:HD2	1.74	0.45
1:D:279:THR:O	1:D:283:ILE:HG13	2.16	0.45
1:D:221:LEU:HB3	1:D:285:VAL:HG21	1.99	0.45
1:E:250:GLY:O	1:E:254:ARG:HB2	2.17	0.45
1:C:119:ILE:HD12	1:C:119:ILE:H	1.81	0.45
1:D:371:TRP:CE2	1:D:420:LEU:HD13	2.52	0.45
1:E:159:ARG:HA	1:E:162:GLU:HG3	1.98	0.45
1:A:418:MET:O	1:A:422:ILE:HG13	2.17	0.45
1:B:127:VAL:HG12	1:B:131:ARG:HD2	1.99	0.45
1:E:55:PHE:CD2	1:E:56:ARG:HG3	2.52	0.45
1:B:225:LEU:HD23	1:B:342:LEU:HD23	1.99	0.44
1:C:68:ILE:HG23	1:C:81:ILE:HG23	1.99	0.44
1:D:27:LEU:HD12	1:D:392:ARG:HG3	1.99	0.44
1:A:277:ARG:HD2	1:A:408:TYR:CE2	2.52	0.44
1:D:275:LEU:HD22	1:D:327:LEU:HD11	1.99	0.44
1:A:19:LEU:HB2	1:A:37:ILE:HG23	1.98	0.44
1:C:113:LEU:HD21	1:C:152:ILE:HG12	1.98	0.44
1:E:26:LEU:HD13	1:E:318:VAL:HG22	1.98	0.44
1:A:306:TYR:CE1	1:A:345:TYR:HA	2.53	0.44
1:C:418:MET:O	1:C:422:ILE:HG13	2.18	0.44
1:C:434:PRO:O	1:C:438:LYS:HG3	2.16	0.44
1:A:205:CYS:HB3	1:A:339:ARG:HD3	1.98	0.43
1:B:205:CYS:HB3	1:B:339:ARG:HD3	1.99	0.43
1:B:426:ALA:O	1:B:430:THR:OG1	2.28	0.43
1:C:237:ALA:HB3	1:C:238:PRO:HD3	2.00	0.43
1:D:446:ASP:HB2	1:D:450:LYS:HE3	2.00	0.43
1:C:302:ILE:HB	1:C:439:PHE:CD2	2.48	0.43
1:A:52:HIS:HB2	1:A:94:PRO:O	2.18	0.43
1:E:434:PRO:O	1:E:438:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:PHE:HZ	1:C:129:PHE:CZ	2.36	0.43
1:A:320:ILE:HA	1:A:330:ARG:HD2	2.00	0.43
1:D:205:CYS:SG	1:D:339:ARG:HD3	2.58	0.43
1:E:277:ARG:HD2	1:E:408:TYR:CE2	2.53	0.43
1:C:288:TYR:CD1	1:C:413:PRO:HB2	2.54	0.43
1:B:17:ILE:HD12	1:B:44:LEU:HB3	2.01	0.43
1:E:171:LEU:HD12	1:E:183:ILE:HG23	2.01	0.43
1:A:434:PRO:O	1:A:438:LYS:HG3	2.19	0.42
1:C:102:THR:O	1:C:106:LEU:HG	2.18	0.42
1:D:356:ASP:OD1	1:D:356:ASP:N	2.49	0.42
1:E:443:THR:HA	1:E:449:TRP:HE1	1.84	0.42
1:A:27:LEU:HB3	1:A:29:ASP:OD2	2.19	0.42
1:A:237:ALA:HB3	1:A:238:PRO:HD3	2.00	0.42
1:B:17:ILE:HG12	1:B:181:SER:OG	2.18	0.42
1:D:68:ILE:HD11	1:D:85:TYR:HB2	2.00	0.42
1:D:278:ARG:HA	1:D:278:ARG:HD2	1.84	0.42
1:C:55:PHE:CD2	1:C:56:ARG:HG3	2.55	0.42
1:C:277:ARG:NH2	1:C:278:ARG:HD3	2.34	0.42
1:D:307:MET:HE1	1:D:386:HIS:HB3	2.01	0.42
1:E:301:LYS:HD3	1:E:429:THR:HB	2.01	0.42
1:C:211:ILE:HG13	1:C:211:ILE:H	1.52	0.42
1:A:206:GLU:CD	1:A:336:TRP:HE1	2.22	0.42
1:C:181:SER:O	1:C:185:GLU:HG3	2.20	0.42
1:D:19:LEU:H	1:D:41:ASN:ND2	2.16	0.42
1:D:146:VAL:O	1:D:153:ALA:HB1	2.20	0.42
1:E:211:ILE:H	1:E:211:ILE:HG13	1.48	0.42
1:A:56:ARG:HH22	1:A:59:ALA:HB3	1.84	0.42
1:A:56:ARG:NH2	1:A:59:ALA:HB3	2.35	0.42
1:D:144:LYS:HE3	1:D:145:TYR:CE2	2.55	0.42
1:B:237:ALA:HB3	1:B:238:PRO:HD3	2.02	0.42
1:D:51:TRP:HB3	1:D:92:GLN:HG3	2.02	0.42
1:B:307:MET:HE1	1:B:386:HIS:HB3	2.02	0.41
1:C:320:ILE:HA	1:C:330:ARG:HD2	2.01	0.41
1:B:323:ASP:OD1	1:B:323:ASP:N	2.52	0.41
1:D:306:TYR:HE1	1:D:345:TYR:HA	1.84	0.41
1:E:211:ILE:O	1:E:213:TYR:HD1	2.02	0.41
1:A:116:LEU:HD12	1:A:155:LYS:NZ	2.35	0.41
1:D:418:MET:O	1:D:422:ILE:HG13	2.21	0.41
1:E:288:TYR:CD1	1:E:413:PRO:HB2	2.55	0.41
1:C:205:CYS:HB3	1:C:339:ARG:HD3	2.02	0.41
1:C:306:TYR:O	1:C:309:THR:OG1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:LEU:HD13	1:D:318:VAL:HG22	2.03	0.41
1:B:434:PRO:O	1:B:438:LYS:HG3	2.21	0.41
1:E:85:TYR:O	1:E:89:VAL:HB	2.21	0.41
1:A:17:ILE:HG12	1:A:181:SER:OG	2.20	0.41
1:A:250:GLY:O	1:A:254:ARG:HB2	2.20	0.41
1:B:56:ARG:HH22	1:B:59:ALA:HB3	1.86	0.41
1:B:243:PHE:CE1	1:C:208:GLN:HB3	2.56	0.41
1:C:250:GLY:O	1:C:254:ARG:HB2	2.20	0.41
1:A:288:TYR:CD1	1:A:413:PRO:HB2	2.56	0.41
1:D:318:VAL:O	1:D:322:GLN:HG2	2.20	0.41
1:E:61:HIS:CE1	1:E:166:HIS:HD1	2.38	0.41
1:E:218:PRO:HB2	1:E:278:ARG:HH12	1.86	0.41
1:A:277:ARG:NH2	1:A:278:ARG:HD3	2.36	0.41
1:B:155:LYS:HE2	1:B:155:LYS:HB3	1.94	0.41
1:B:159:ARG:HA	1:B:162:GLU:HG3	2.03	0.41
1:C:48:HIS:CE1	1:C:181:SER:HB2	2.55	0.41
1:C:51:TRP:HB3	1:C:92:GLN:HG3	2.01	0.41
1:C:169:ILE:HG12	1:C:315:PHE:HD2	1.83	0.41
1:C:304:PHE:N	1:C:440:VAL:O	2.49	0.41
1:A:310:LEU:HD21	1:A:394:LEU:HG	2.03	0.41
1:A:389:KCX:HE2	1:A:389:KCX:HB3	1.75	0.40
1:B:310:LEU:HD21	1:B:394:LEU:HG	2.02	0.40
1:D:252:VAL:O	1:D:256:LEU:HB2	2.21	0.40
1:E:146:VAL:O	1:E:153:ALA:HB1	2.22	0.40
1:B:395:LYS:O	1:B:399:GLU:HG2	2.20	0.40
1:A:102:THR:O	1:A:106:LEU:HG	2.21	0.40
1:A:202:PHE:CZ	1:A:340:LEU:HD22	2.57	0.40
1:A:294:GLN:OE1	1:A:301:LYS:N	2.45	0.40
1:C:277:ARG:HD2	1:C:408:TYR:CZ	2.56	0.40
1:B:327:LEU:HD12	1:B:327:LEU:HA	1.89	0.40
1:D:213:TYR:HA	1:D:214:PRO:HA	1.89	0.40
1:D:354:HIS:HB2	1:D:356:ASP:OD1	2.21	0.40
1:A:279:THR:O	1:A:283:ILE:HG13	2.22	0.40
1:A:398:GLN:HG3	1:A:419:TRP:CD1	2.56	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	443/456 (97%)	410 (93%)	31 (7%)	2 (0%)	25	59
1	B	443/456 (97%)	417 (94%)	23 (5%)	3 (1%)	19	53
1	C	443/456 (97%)	416 (94%)	24 (5%)	3 (1%)	19	53
1	D	443/456 (97%)	414 (94%)	25 (6%)	4 (1%)	14	48
1	E	443/456 (97%)	417 (94%)	23 (5%)	3 (1%)	19	53
All	All	2215/2280 (97%)	2074 (94%)	126 (6%)	15 (1%)	19	53

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	GLY
1	E	250	GLY
1	A	214	PRO
1	C	214	PRO
1	D	214	PRO
1	D	442	PHE
1	D	250	GLY
1	B	215	PRO
1	B	250	GLY
1	C	215	PRO
1	D	251	VAL
1	C	250	GLY
1	E	215	PRO
1	E	214	PRO
1	B	214	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	359/366 (98%)	324 (90%)	35 (10%)	6	28
1	B	359/366 (98%)	325 (90%)	34 (10%)	7	29
1	C	359/366 (98%)	320 (89%)	39 (11%)	5	25
1	D	359/366 (98%)	319 (89%)	40 (11%)	5	24
1	E	359/366 (98%)	322 (90%)	37 (10%)	6	26
All	All	1795/1830 (98%)	1610 (90%)	185 (10%)	6	26

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	23	HIS
1	A	24	VAL
1	A	29	ASP
1	A	58	ARG
1	A	89	VAL
1	A	91	ILE
1	A	98	VAL
1	A	105	ARG
1	A	131	ARG
1	A	143	ASN
1	A	148	SER
1	A	150	ASN
1	A	178	GLN
1	A	193	HIS
1	A	199	SER
1	A	211	ILE
1	A	217	HIS
1	A	245	ASN
1	A	254	ARG
1	A	295	ARG
1	A	301	LYS
1	A	302	ILE
1	A	314	LEU
1	A	323	ASP
1	A	352	GLU
1	A	354	HIS
1	A	358	ILE

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Mol	Chain	Res	Type
1	A	364	ASP
1	A	378	VAL
1	A	384	ASP
1	A	410	ASP
1	A	436	ASP
1	A	446	ASP
1	A	451	ILE
1	B	11	VAL
1	B	21	ASP
1	B	23	HIS
1	B	24	VAL
1	B	58	ARG
1	B	91	ILE
1	B	98	VAL
1	B	105	ARG
1	B	143	ASN
1	B	155	LYS
1	B	178	GLN
1	B	193	HIS
1	B	195	ASP
1	B	199	SER
1	B	211	ILE
1	B	217	HIS
1	B	289	MET
1	B	301	LYS
1	B	314	LEU
1	B	323	ASP
1	B	326	SER
1	B	352	GLU
1	B	354	HIS
1	B	358	ILE
1	B	364	ASP
1	B	378	VAL
1	B	384	ASP
1	B	408	TYR
1	B	410	ASP
1	B	417	ASP
1	B	421	LYS
1	B	436	ASP
1	B	446	ASP
1	B	451	ILE
1	C	11	VAL

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Mol	Chain	Res	Type
1	C	24	VAL
1	C	52	HIS
1	C	58	ARG
1	C	89	VAL
1	C	91	ILE
1	C	92	GLN
1	C	98	VAL
1	C	105	ARG
1	C	136	HIS
1	C	143	ASN
1	C	156	MET
1	C	170	HIS
1	C	178	GLN
1	C	199	SER
1	C	211	ILE
1	C	217	HIS
1	C	245	ASN
1	C	254	ARG
1	C	274	GLU
1	C	289	MET
1	C	295	ARG
1	C	300	ARG
1	C	301	LYS
1	C	302	ILE
1	C	307	MET
1	C	314	LEU
1	C	323	ASP
1	C	352	GLU
1	C	354	HIS
1	C	358	ILE
1	C	364	ASP
1	C	378	VAL
1	C	384	ASP
1	C	408	TYR
1	C	410	ASP
1	C	421	LYS
1	C	436	ASP
1	C	451	ILE
1	D	11	VAL
1	D	21	ASP
1	D	23	HIS
1	D	24	VAL

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Mol	Chain	Res	Type
1	D	29	ASP
1	D	52	HIS
1	D	58	ARG
1	D	89	VAL
1	D	91	ILE
1	D	98	VAL
1	D	105	ARG
1	D	131	ARG
1	D	136	HIS
1	D	143	ASN
1	D	170	HIS
1	D	178	GLN
1	D	205	CYS
1	D	211	ILE
1	D	217	HIS
1	D	245	ASN
1	D	254	ARG
1	D	282	MET
1	D	289	MET
1	D	295	ARG
1	D	323	ASP
1	D	350	SER
1	D	352	GLU
1	D	354	HIS
1	D	358	ILE
1	D	364	ASP
1	D	372	LYS
1	D	378	VAL
1	D	384	ASP
1	D	408	TYR
1	D	410	ASP
1	D	417	ASP
1	D	421	LYS
1	D	436	ASP
1	D	446	ASP
1	D	451	ILE
1	E	11	VAL
1	E	16	GLN
1	E	21	ASP
1	E	23	HIS
1	E	24	VAL
1	E	29	ASP

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Mol	Chain	Res	Type
1	E	58	ARG
1	E	89	VAL
1	E	91	ILE
1	E	92	GLN
1	E	98	VAL
1	E	105	ARG
1	E	143	ASN
1	E	155	LYS
1	E	170	HIS
1	E	178	GLN
1	E	193	HIS
1	E	199	SER
1	E	211	ILE
1	E	217	HIS
1	E	254	ARG
1	E	282	MET
1	E	289	MET
1	E	302	ILE
1	E	323	ASP
1	E	352	GLU
1	E	354	HIS
1	E	358	ILE
1	E	364	ASP
1	E	378	VAL
1	E	384	ASP
1	E	408	TYR
1	E	410	ASP
1	E	436	ASP
1	E	443	THR
1	E	446	ASP
1	E	451	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	92	GLN
1	A	139	GLN
1	B	14	ASN
1	B	92	GLN
1	B	139	GLN
1	C	14	ASN

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Mol	Chain	Res	Type
1	C	45	GLN
1	C	92	GLN
1	C	139	GLN
1	C	150	ASN
1	D	14	ASN
1	D	41	ASN
1	D	139	GLN
1	D	398	GLN
1	E	14	ASN
1	E	92	GLN
1	E	139	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

5 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	$\#\|Z\| > 2$
1	KCX	A	389	1,2	9,11,12	0.92	0	5,12,14	1.43	1 (20%)
1	KCX	E	389	1,2	9,11,12	1.13	1 (11%)	5,12,14	1.82	2 (40%)
1	KCX	D	389	1	9,11,12	0.95	0	5,12,14	1.49	1 (20%)
1	KCX	B	389	1,2	9,11,12	1.20	1 (11%)	5,12,14	1.72	2 (40%)
1	KCX	C	389	1,2	9,11,12	0.94	0	5,12,14	1.51	1 (20%)

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
1	KCX	A	389	1,2	-	3/9/10/12	-
1	KCX	E	389	1,2	-	3/9/10/12	-
1	KCX	D	389	1	-	2/9/10/12	-
1	KCX	B	389	1,2	-	3/9/10/12	-
1	KCX	C	389	1,2	-	3/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	389	KCX	OQ1-CX	2.56	1.26	1.21
1	E	389	KCX	OQ1-CX	2.37	1.26	1.21

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	389	KCX	OQ1-CX-NZ	-3.33	119.79	124.96
1	C	389	KCX	OQ1-CX-NZ	-2.91	120.45	124.96
1	B	389	KCX	OQ1-CX-NZ	-2.86	120.53	124.96
1	D	389	KCX	OQ1-CX-NZ	-2.70	120.77	124.96
1	A	389	KCX	OQ1-CX-NZ	-2.56	120.99	124.96
1	B	389	KCX	CE-NZ-CX	-2.25	118.28	121.89
1	E	389	KCX	CE-NZ-CX	-2.19	118.36	121.89

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	389	KCX	O-C-CA-CB
1	E	389	KCX	CE-CD-CG-CB
1	E	389	KCX	CG-CD-CE-NZ
1	A	389	KCX	CE-CD-CG-CB
1	B	389	KCX	CE-CD-CG-CB
1	C	389	KCX	CA-CB-CG-CD
1	A	389	KCX	CA-CB-CG-CD
1	C	389	KCX	CE-CD-CG-CB
1	D	389	KCX	CA-CB-CG-CD
1	A	389	KCX	N-CA-CB-CG
1	C	389	KCX	N-CA-CB-CG
1	D	389	KCX	CE-CD-CG-CB
1	B	389	KCX	CA-CB-CG-CD
1	B	389	KCX	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	389	KCX	2	0
1	C	389	KCX	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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, 95^{th} 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	445/456 (97%)	-0.10	6 (1%)	74	53	56, 88, 118, 149	0
1	B	445/456 (97%)	-0.13	2 (0%)	89	75	58, 95, 130, 150	0
1	C	445/456 (97%)	-0.19	2 (0%)	89	75	58, 93, 131, 152	0
1	D	445/456 (97%)	0.22	11 (2%)	58	39	79, 109, 135, 154	0
1	E	445/456 (97%)	-0.10	4 (0%)	81	61	79, 104, 134, 156	0
All	All	2225/2280 (97%)	-0.06	25 (1%)	77	57	56, 99, 132, 156	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	213	TYR	5.6
1	D	262	ILE	3.2
1	A	11	VAL	3.0
1	D	221	LEU	2.9
1	D	422	ILE	2.9
1	D	368	ASP	2.8
1	D	266	PHE	2.8
1	C	383	ASP	2.7
1	D	11	VAL	2.7
1	A	21	ASP	2.6
1	E	119	ILE	2.6
1	E	138	TRP	2.5
1	A	378	VAL	2.5
1	D	13	LEU	2.5
1	D	423	ALA	2.4
1	C	57	ASP	2.4
1	D	369	MET	2.3
1	B	366	SER	2.3
1	A	355	ASP	2.2
1	B	213	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	414	VAL	2.1
1	D	344	TRP	2.1
1	A	13	LEU	2.1
1	E	165	TYR	2.0
1	D	24	VAL	2.0

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, 95^{th} 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
1	KCX	B	389	12/13	0.93	0.23	78,90,105,115	0
1	KCX	A	389	12/13	0.95	0.12	63,76,81,82	0
1	KCX	D	389	12/13	0.95	0.17	97,106,113,114	0
1	KCX	E	389	12/13	0.96	0.11	87,95,103,110	0
1	KCX	C	389	12/13	0.98	0.10	66,71,78,79	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	FE	B	501	1/1	0.94	0.11	126,126,126,126	0
2	FE	D	501	1/1	0.95	0.07	83,83,83,83	0
2	FE	C	501	1/1	0.96	0.06	76,76,76,76	0
2	FE	E	501	1/1	0.98	0.09	117,117,117,117	0
2	FE	A	501	1/1	1.00	0.02	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.