



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:28 AM UTC

PDB ID : 4CCG / pdb_00004ccg
Title : Structure of an E2-E3 complex
Authors : Hodson, C.; Purkiss, A.; Walden, H.
Deposited on : 2013-10-22
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

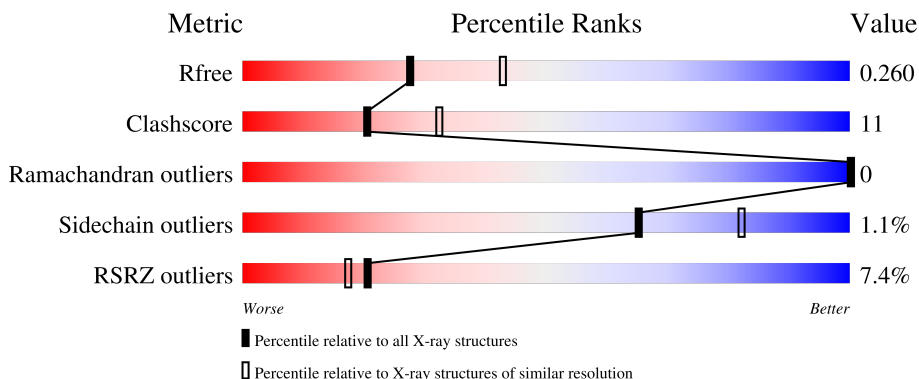
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	212	5% (Poor fit) 56% (0 outliers) 18% (1 outlier) 26% (2+ outliers)
1	B	212	3% (Poor fit) 54% (0 outliers) 15% (1 outlier) 31% (2+ outliers)
2	X	88	2% (Poor fit) 75% (0 outliers) 10% (1 outlier) 15% (2+ outliers)
2	Y	88	16% (Poor fit) 63% (0 outliers) 14% (1 outlier) 24% (2+ outliers)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EPE	A	1154[A]	-	-	X	-
4	GOL	A	1157	-	-	X	-

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 3744 atoms, of which 40 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 UBIQUITIN-CONJUGATING ENZYME E2 T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	157	1247	805	211	224	7	0	3	0
1	B	147	1154	751	204	194	5	0	4	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	THR	-	expression tag	UNP Q9NW38
A	-13	GLY	-	expression tag	UNP Q9NW38
A	-12	SER	-	expression tag	UNP Q9NW38
A	-11	THR	-	expression tag	UNP Q9NW38
A	-10	GLY	-	expression tag	UNP Q9NW38
A	-9	SER	-	expression tag	UNP Q9NW38
A	-8	THR	-	expression tag	UNP Q9NW38
A	-7	GLY	-	expression tag	UNP Q9NW38
A	-6	GLU	-	expression tag	UNP Q9NW38
A	-5	ASN	-	expression tag	UNP Q9NW38
A	-4	LEU	-	expression tag	UNP Q9NW38
A	-3	TYR	-	expression tag	UNP Q9NW38
A	-2	THR	-	expression tag	UNP Q9NW38
A	-1	GLN	-	expression tag	UNP Q9NW38
A	0	GLY	-	expression tag	UNP Q9NW38
B	-14	THR	-	expression tag	UNP Q9NW38
B	-13	GLY	-	expression tag	UNP Q9NW38
B	-12	SER	-	expression tag	UNP Q9NW38
B	-11	THR	-	expression tag	UNP Q9NW38
B	-10	GLY	-	expression tag	UNP Q9NW38
B	-9	SER	-	expression tag	UNP Q9NW38
B	-8	THR	-	expression tag	UNP Q9NW38
B	-7	GLY	-	expression tag	UNP Q9NW38
B	-6	GLU	-	expression tag	UNP Q9NW38
B	-5	ASN	-	expression tag	UNP Q9NW38

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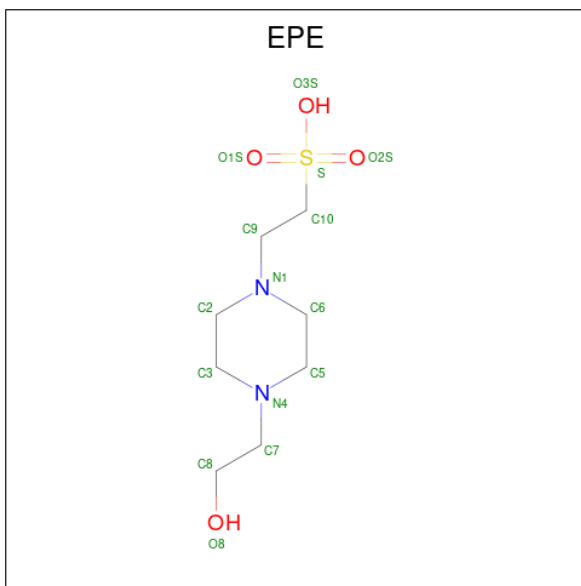
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	LEU	-	expression tag	UNP Q9NW38
B	-3	TYR	-	expression tag	UNP Q9NW38
B	-2	THR	-	expression tag	UNP Q9NW38
B	-1	GLN	-	expression tag	UNP Q9NW38
B	0	GLY	-	expression tag	UNP Q9NW38

- Molecule 2 is a protein called E3 UBIQUITIN-PROTEIN LIGASE FANCL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	X	75	Total	C	N	O	S	0	4	0
			614	389	100	116	9			
2	Y	67	Total	C	N	O	S	0	0	0
			512	328	80	95	9			

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



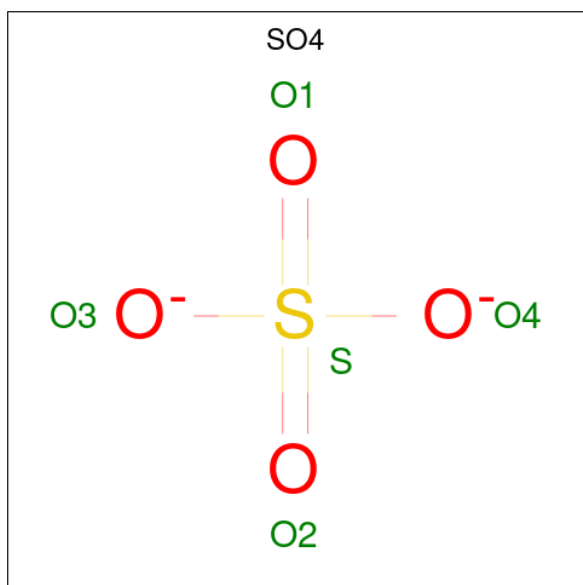
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
3	A	1	Total	C	N	O	S	0	1	
			15	8	2	4	1			
3	A	1	Total	C	H	N	O	S	0	0
			11	2	4	1	3	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	14	3	8	3	0	0
4	A	1	14	3	8	3	0	0
4	B	1	14	3	8	3	0	0
4	X	1	14	3	8	3	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	1
5	Y	1	Total O S 5 4 1	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Cl 1 1	0	0

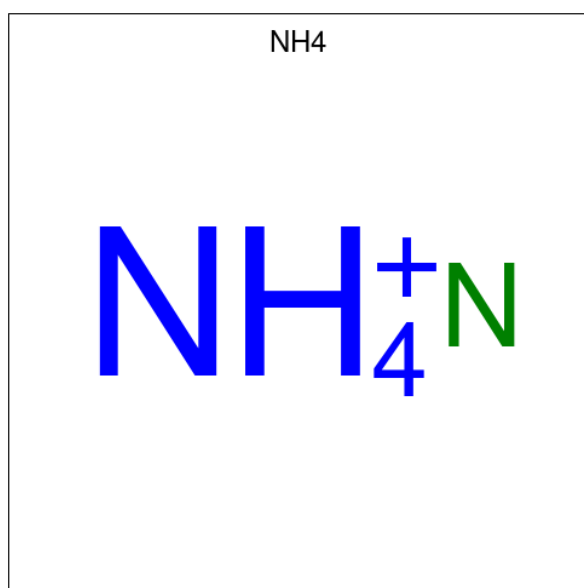
- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Na 1 1	0	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	X	2	Total Zn 2 2	0	0
8	Y	2	Total Zn 2 2	0	0

- Molecule 9 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	X	1	Total	H	N	0	0
			5	4	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	66	Total	O	0	0
			66	66		
10	B	23	Total	O	0	0
			23	23		
10	X	22	Total	O	0	0
			22	22		
10	Y	3	Total	O	0	0
			3	3		



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.22Å 109.22Å 117.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.82 – 2.40 46.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.82-2.40) 94.4 (46.82-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.34Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.212 , 0.248 0.227 , 0.260	Depositor DCC
R_{free} test set	1518 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtrriage
Anisotropy	0.264	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3744	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: EPE, ZN, NA, CL, NH4, SO4, GOL

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	0.32	0/1288	0.73	0/1758
1	B	0.30	0/1199	0.77	0/1638
2	X	0.28	0/639	0.65	0/862
2	Y	0.27	0/524	0.72	0/710
All	All	0.30	0/3650	0.73	0/4968

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1247	0	1228	39	0
1	B	1154	0	1156	26	0
2	X	614	0	580	9	0
2	Y	512	0	467	10	0
3	A	22	4	23	12	0
4	A	12	16	16	5	0
4	B	6	8	7	0	0
4	X	6	8	8	0	0
5	A	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Y	5	0	0	0	0
6	B	1	0	0	0	0
7	B	1	0	0	0	0
8	X	2	0	0	0	0
8	Y	2	0	0	0	0
9	X	1	4	0	0	0
10	A	66	0	0	1	0
10	B	23	0	0	0	0
10	X	22	0	0	0	0
10	Y	3	0	0	0	0
All	All	3704	40	3485	79	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 11.

The worst 5 of 79 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ARG:HH21	3:A:1154[A]:EPE:H81	1.46	0.81
2:X:316:ASP:OD2	2:X:373[A]:ARG:NH1	2.18	0.76
1:B:13:MET:HA	1:B:16[B]:THR:HG22	1.68	0.75
1:A:-2:THR:H	1:A:1:MET:HE3	1.55	0.70
1:A:34:LEU:HB2	1:A:55:VAL:HB	1.76	0.67

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	158/212 (74%)	154 (98%)	4 (2%)	0	100	100
1	B	147/212 (69%)	146 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	76/88 (86%)	72 (95%)	4 (5%)	0	100	100
2	Y	63/88 (72%)	61 (97%)	2 (3%)	0	100	100
All	All	444/600 (74%)	433 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	131/186 (70%)	129 (98%)	2 (2%)	57	77
1	B	118/186 (63%)	117 (99%)	1 (1%)	73	86
2	X	69/79 (87%)	68 (99%)	1 (1%)	59	79
2	Y	55/79 (70%)	55 (100%)	0	100	100
All	All	373/530 (70%)	369 (99%)	4 (1%)	65	82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	31	MET
1	B	136	LYS
2	X	299	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	150	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 6 are monoatomic and 1 is modelled with single atom - leaving 8 for Mogul analysis.

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
4	GOL	A	1157	-	5,5,5	0.36	0	5,5,5	0.21	0
4	GOL	A	1156	-	5,5,5	0.35	0	5,5,5	0.38	0
3	EPE	A	1155	-	6,6,15	3.22	1 (16%)	7,8,20	1.65	1 (14%)
5	SO4	A	1158[B]	-	4,4,4	0.24	0	6,6,6	0.09	0
3	EPE	A	1154[A]	-	15,15,15	2.08	1 (6%)	19,20,20	2.82	12 (63%)
4	GOL	X	1376	-	5,5,5	0.35	0	5,5,5	0.26	0
4	GOL	B	1154	7	5,5,5	0.38	0	5,5,5	0.20	0
5	SO4	Y	1374	-	4,4,4	0.24	0	6,6,6	0.08	0

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
4	GOL	A	1157	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	1156	-	-	2/4/4/4	-
3	EPE	A	1155	-	-	0/4/4/19	-
3	EPE	A	1154[A]	-	-	3/9/19/19	0/1/1/1
4	GOL	X	1376	-	-	2/4/4/4	-
4	GOL	B	1154	7	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1154[A]	EPE	C10-S	-7.74	1.66	1.77
3	A	1155	EPE	C10-S	-7.69	1.66	1.77

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1154[A]	EPE	C6-N1-C2	5.24	120.13	108.84
3	A	1154[A]	EPE	C5-N4-C3	4.88	119.35	108.84
3	A	1154[A]	EPE	C7-N4-C5	3.44	120.40	111.24
3	A	1154[A]	EPE	C7-N4-C3	3.38	120.25	111.24
3	A	1154[A]	EPE	C6-C5-N4	-3.30	104.00	110.65

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1154[A]	EPE	C10-C9-N1-C2
4	A	1157	GOL	O1-C1-C2-C3
4	B	1154	GOL	C1-C2-C3-O3
4	X	1376	GOL	C1-C2-C3-O3
3	A	1154[A]	EPE	C8-C7-N4-C3

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1157	GOL	4	0
4	A	1156	GOL	1	0
3	A	1155	EPE	3	0
5	A	1158[B]	SO4	1	0
3	A	1154[A]	EPE	9	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	157/212 (74%)	0.15	10 (6%) 25 22	23, 47, 84, 116	3 (1%)
1	B	147/212 (69%)	0.46	7 (4%) 35 32	32, 65, 86, 114	4 (2%)
2	X	75/88 (85%)	0.11	2 (2%) 56 52	31, 47, 75, 89	4 (5%)
2	Y	67/88 (76%)	1.15	14 (20%) 2 2	52, 72, 101, 124	0
All	All	446/600 (74%)	0.40	33 (7%) 20 17	23, 59, 91, 124	11 (2%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	351	SER	10.0
2	Y	303	PHE	5.1
2	Y	350	GLN	4.4
2	Y	371	SER	4.3
1	B	0	GLY	4.1

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

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

6.3 Carbohydrates [i](#)

There are no 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(\AA^2)	Q<0.9
3	EPE	A	1155	7/15	0.45	0.14	87,110,145,146	0
4	GOL	A	1156	6/6	0.55	0.23	75,90,99,102	0
5	SO4	Y	1374	5/5	0.59	0.12	147,148,149,149	0
4	GOL	A	1157	6/6	0.61	0.27	72,86,99,99	0
4	GOL	B	1154	6/6	0.69	0.17	80,96,100,100	0
3	EPE	A	1154[A]	15/15	0.69	0.28	40,70,96,96	15
4	GOL	X	1376	6/6	0.78	0.17	64,77,90,91	0
9	NH4	X	1377	1/1	0.83	0.13	67,80,80,80	0
5	SO4	A	1158[B]	5/5	0.87	0.17	89,92,93,93	5
7	NA	B	1155	1/1	0.90	0.22	65,65,65,65	0
6	CL	B	1153	1/1	0.97	0.07	72,72,72,72	0
8	ZN	Y	1372	1/1	0.99	0.03	63,63,63,63	0
8	ZN	X	1374	1/1	1.00	0.03	38,38,38,38	0
8	ZN	Y	1373	1/1	1.00	0.02	57,57,57,57	0
8	ZN	X	1375	1/1	1.00	0.04	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.